Solubility Data

1. $CHBrCl_2$
Bromodichloromethane
Dichlorobromomethane
BDCM
RN: 75-27-4 **MP** (°C)**:** –55
MW: 163.83 **BP** (°C)**:** 87

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	3.032E+00	30	M300	1 1 2 2 2	
1.812E-02	2.968E+00	30	M311	1 1 2 2 2	

2. $CHBr_2Cl$
Chlorodibromomethane
Dibromochloromethane
CDBM
RN: 124-48-1 **MP** (°C)**:** –22
MW: 208.29 **BP** (°C)**:** 119.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E-03	1.050E+00	30	M300	1 1 2 2 2	
1.205E-02	2.509E+00	30	M311	1 1 2 2 2	

3. $CHBr_3$
Bromoform
Tribromomethane
Methyl tribromide
RN: 75-25-2 **MP** (°C)**:** 7.5
MW: 252.75 BP (°C)**:** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	3.001E+00	15	G029	1 0 2 2 2	
3.957E-03	1.000E+00	20	F300	1 0 0 0 0	
<7.91E-04	<2.00E-01	25	B019	1 0 1 2 0	*sic*
1.262E-02	3.190E+00	30	F300	1 0 0 0 2	
1.258E-02	3.180E+00	30	G029	1 0 2 2 2	
1.555E-02	3.931E+00	30	M311	1 1 2 2 2	
1.256E-02	3.174E+00	30	V009	1 0 0 0 2	
1.227E-02	3.100E+00	ns	O006	0 0 0 0 2	

4. $CHClF_2$
Chlorodifluoromethane
Freon 22
Halocarbon 22
RN: 75-45-6 **MP** (°C)**:** –146
MW: 86.47 **BP** (°C)**:** –40.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.018E-01	2.610E+01	21	M065	1 0 2 1 2	

5. $CHCl_3$
Chloroform
Trichloromethane
Methyl trichloride
Formyl trichloride
RN: 67-66-3 **MP** (°C)**:** –63
MW: 119.38 **BP** (°C)**:** 61

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-02	1.062E+01	0	H101	2 0 0 0 2	
7.077E-02	8.448E+00	15	G029	1 0 2 2 2	
7.134E-02	8.517E+00	15	J036	0 0 0 0 0	
6.648E-02	7.937E+00	20	E019	1 0 1 1 0	
6.785E-02	8.100E+00	20	F300	1 0 0 0 1	
6.886E-02	8.220E+00	20	H101	2 0 0 0 2	
6.869E-02	8.200E+00	20	M133	1 0 0 0 2	
6.827E-02	8.150E+00	20	M368	1 0 0 0 1	
6.648E-02	7.937E+00	20	N034	1 0 0 0 0	
6.869E-02	8.200E+00	20	P046	1 0 0 0 0	
6.750E-02	8.058E+00	20	P073	1 0 0 1 2	
3.504E-02	4.182E+00	22	H072	1 0 1 1 2	
7.472E-02	8.920E+00	25	B019	1 0 1 2 0	
6.050E-02	7.222E+00	25	B173	2 0 2 2 2	
6.660E-02	7.950E+00	25	F071	1 1 2 1 2	
6.648E-02	7.937E+00	25	G056	1 0 0 0 2	
6.813E-02	8.133E+00	25	L319	1 0 2 1 2	
6.618E-02	7.900E+00	25	M037	1 1 0 0 1	
6.648E-02	7.937E+00	25	O026	1 2 0 1 0	
7.472E-02	8.920E+00	25	R321	1 2 1 1 1	
6.236E-02	7.444E+00	25.0	C055	1 2 1 0 1	
6.409E-02	7.651E+00	30	G029	1 0 2 2 2	
6.500E-02	7.760E+00	30	H101	2 0 0 0 2	
2.114E-02	2.524E+00	30	M311	1 1 2 2 2	
6.411E-02	7.653E+00	30	V009	1 0 0 0 2	
6.648E-02	7.937E+00	56.1	C055	2 2 1 0 0	
6.236E-02	7.444E+00	60	R321	1 2 1 1 1	
6.660E-02	7.950E+00	ns	H123	0 0 0 0 0	

(*continued*)

5. $CHCl_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.168E-02	4.975E+00	ns	I306	0 0 0 0 0	
6.660E-02	7.950E+00	ns	M344	0 0 0 0 2	
6.830E-02	8.153E+00	ns	R028	0 0 0 0 0	

6. CHI_3

Iodoform
Triiodomethane

RN: 75-47-8 **MP** (°C)**:** 121.5
MW: 393.73 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	1.181E-01	25	V009	1 0 0 0 0	
2.540E-04	9.999E-02	rt	D021	0 0 1 1 0	

7. CH_2BrCl

Bromochloromethane
Bromo-chloro-methane
Chlorobromomethane
CBM

RN: 74-97-5 **MP** (°C)**:** –86.5
MW: 129.39 **BP** (°C)**:** 68.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-01	1.669E+01	25	M342	1 0 1 1 2	
1.142E-01	1.478E+01	ns	O006	0 0 0 0 1	

8. CH_2Br_2

Methylene bromide
Dibrom-methan

RN: 74-95-3 **MP** (°C)**:** –52.7
MW: 173.85 **BP** (°C)**:** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-02	1.173E+01	0	H101	2 0 0 0 2	
6.652E-02	1.156E+01	15	G029	1 0 2 2 2	
6.604E-02	1.148E+01	20	H101	2 0 0 0 2	
6.259E-02	1.088E+01	25	O006	1 0 0 0 1	
6.782E-02	1.179E+01	30	G029	1 0 2 2 2	

(*continued*)

8. CH_2Br_2 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.765E-02	1.176E+01	30	H101	2 0 0 0 2	
6.779E-02	1.179E+01	30	V009	1 0 0 0 2	
6.558E-02	1.140E+01	ns	F300	0 0 0 0 2	

9. CH_2Cl_2

Methylene chloride
Dichlor-methan
Dichloromethane
Methylene dichloride
Methane dichloride

RN: 75-09-2 **MP** (°C)**:** –95.1
MW: 84.93 **BP** (°C)**:** 39.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.782E-01	2.363E+01	0	H101	2 0 0 0 2	
2.309E-01	1.961E+01	20	C057	0 0 0 0 0	
2.355E-01	2.000E+01	20	F300	1 0 0 0 0	
2.355E-01	2.000E+01	20	H101	2 0 0 0 2	
2.263E-01	1.922E+01	20	N034	1 0 0 0 2	
1.887E-01	1.603E+01	20	N038	1 0 0 1 2	
2.309E-01	1.961E+01	25	A094	1 0 0 0 1	
1.534E-01	1.303E+01	25	G056	1 0 0 0 2	
1.554E-01	1.320E+01	25	M037	1 1 0 0 2	
1.554E-01	1.320E+01	25	M133	1 0 0 0 2	
1.554E-01	1.320E+01	25	P046	1 0 0 0 0	
2.275E-01	1.932E+01	30	V009	1 0 0 0 2	
2.284E-01	1.940E+01	ns	H123	0 0 0 0 0	

10. CH_2I_2

Methylene iodide
Diiod-methan

RN: 75-11-6 **MP** (°C)**:** 6.0
MW: 267.84 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-03	8.330E-01	25	A032	1 2 1 1 2	
4.624E-03	1.238E+00	30	G029	1 0 2 2 2	
4.594E-03	1.231E+00	30	V009	1 0 0 0 1	

11. CH_2N_2
Cyanamide
Cyanamid
RN: 420-04-2 **MP** (°C)**:**
MW: 42.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E+01	4.444E+02	ns	N013	0 0 0 0 1	

12. CH_3Br
Methyl bromide
Bromomethane
Celfume
RN: 74-83-9 **MP** (°C)**:** –94
MW: 94.94 **BP** (°C)**:** 3.56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-01	2.609E+01	10	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	M061	1 0 0 0 2	
1.933E-01	1.835E+01	19.9	G061	1 2 1 1 2	774.3mm Hg @ 25 °C
1.685E-01	1.600E+01	20	G080	1 0 0 0 1	
1.659E-01	1.575E+01	20	P081	1 0 0 0 1	
1.394E-01	1.323E+01	25	H081	1 0 2 0 2	
1.411E-01	1.340E+01	25	M161	1 0 0 0 2	
1.196E-01	1.136E+01	32	H081	1 0 2 0 2	
9.479E-03	9.000E-01	ns	N013	0 0 0 0 1	

13. $CH_3BrO_6S_2$
Bromomethionic acid
Methanedisulfonic acid, bromo-
RN: 187610-86-2 **MP** (°C)**:**
MW: 255.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.039E+00	7.752E+02	25	B077	1 2 0 0 2	

14. CH_3Cl

Methyl chloride
Chloromethane

RN: 74-87-3 **MP** (°C)**:** –97.0
MW: 50.49 **BP** (°C)**:** –23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+01	7.727E+02	0	M061	1 0 0 0 1	*sic*
1.436E-01	7.250E+00	20	M133	1 0 0 0 2	
9.069E-02	4.579E+00	20	N034	1 0 0 0 1	
1.436E-01	7.250E+00	20	P046	1 0 0 0 0	
1.059E-01	5.347E+00	24.9	G061	1 2 1 1 2	756.1mm Hg @ 25 °C
1.455E-01	7.346E+00	30	G056	1 0 0 0 2	
1.466E-01	7.400E+00	30	M037	1 1 0 0 1	

15. $CH_3ClO_6S_2$

Chloromethionic acid
Acide chloromethionique

RN: 74692-14-1 **MP** (°C)**:**
MW: 210.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.540E+01	3.243E+03	25	B075	1 2 0 0 2	

16. CH_3F

Fluoromethane
Methylfluoride

RN: 593-53-3 **MP** (°C)**:** –141.8
MW: 34.03 **BP** (°C)**:** –78.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~7.05E-02	~2.40E+00	15	F300	1 0 0 0 0	
5.250E-02	1.787E+00	29.9	G061	1 2 1 1 2	766.8mm Hg @25 °C

17. CH_3I
Iodomethane
Methyl-iodide
Halon 10001
Methyl iodine
Methyliodide
RN: 74-88-4 **MP** (°C)**:** –64
MW: 141.94 **BP** (°C)**:** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-01	1.565E+01	0	H101	2 0 0 0 2	
9.997E-02	1.419E+01	20	H101	2 0 0 0 2	
9.727E-02	1.381E+01	20	H127	1 0 0 0 1	
9.727E-02	1.381E+01	20	I316	0 0 0 0 0	
9.600E-02	1.363E+01	20	M171	1 0 0 0 2	
9.590E-02	1.361E+01	22	F001	1 0 1 2 2	
9.511E-02	1.350E+01	22	F300	1 0 0 0 2	
9.590E-02	1.361E+01	22	S006	1 0 0 0 2	
1.007E-01	1.429E+01	30	H101	2 0 0 0 2	
9.957E-02	1.413E+01	30	V009	1 0 0 0 2	
8.725E-03	1.238E+00	ns	O006	0 0 0 0 1	

18. CH_3NO
Formaldehyde oxime
Formaldehyd-oxim
RN: 75-17-2 **MP** (°C)**:**
MW: 45.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.774E+00	1.700E+02	20	F300	1 0 0 0 1	

19. CH_3NO_2
Nitromethane
Nitrocarbol
NM
RN: 75-52-5 **MP** (°C)**:** –29
MW: 61.04 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E+00	8.676E+01	20	C121	0 0 0 0 1	unit assumed, *sic*
1.627E+00	9.934E+01	25	F049	2 0 2 0 0	
1.802E+00	1.100E+02	25	M136	2 0 0 0 2	
1.802E+00	1.100E+02	25	M139	2 0 0 0 2	
3.039E-01	1.855E+01	ns	D348	0 0 0 0 0	

20. CH_3N_5
5-Aminotetrazole
5-Amino-tetrazol
RN: 4418-61-5 **MP** (°C)**:** 204
MW: 85.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.411E-01	1.200E+01	18	F300	1 0 0 0 1	

21. CH_4
Methane
Methan
RN: 74-82-8 **MP** (°C)**:** –183
MW: 16.04 **BP** (°C)**:** –161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.468E-03	3.960E-02	0	F300	1 0 0 0 2	
2.210E-03	3.545E-02	4.99	C115	2 0 2 2 2	
1.926E-03	3.090E-02	9.99	C115	2 0 2 2 2	
1.633E-03	2.620E-02	14.99	C115	2 0 2 2 2	
1.567E-03	2.513E-02	19.8	G058	1 0 0 0 2	
1.511E-03	2.424E-02	19.99	C115	2 0 2 2 2	
1.446E-03	2.320E-02	20	F300	1 0 0 0 2	
1.381E-03	2.215E-02	24.99	C115	2 0 2 2 2	
1.521E-03	2.440E-02	25	M001	2 1 2 2 2	
1.521E-03	2.440E-02	25	M002	2 2 1 2 2	
1.502E-03	2.410E-02	25	M040	1 0 0 1 2	
1.550E-03	2.487E-02	25	M102	1 2 2 1 2	
1.266E-03	2.030E-02	29.99	C115	2 0 2 2 2	
1.189E-03	1.907E-02	34.99	C115	2 0 2 2 2	
1.079E-03	1.732E-02	39.99	C115	2 0 2 2 2	
1.056E-03	1.693E-02	40	S212	2 1 2 2 2	
1.055E-03	1.693E-02	44.99	C115	2 0 2 2 2	
8.477E-04	1.360E-02	50	F300	1 0 0 0 2	
9.000E-04	1.444E-02	60	S212	2 1 2 2 2	
8.000E-04	1.283E-02	80	S212	2 1 2 2 2	
1.434E-03	2.300E-02	ns	M091	0 1 0 0 2	
1.378E-03	2.210E-02	ns	S212	2 1 2 2 2	

22. CH_4N_2O

Urea
Harnstoff
Uree

RN: 57-13-6 **MP** (°C)**:** 132.7
MW: 60.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E+00	4.012E+02	0	F300	1 0 0 0 2	
4.757E+00	2.857E+02	0	J021	1 0 0 0 2	
6.680E+00	4.012E+02	0	M043	1 0 0 0 1	
6.680E+00	4.012E+02	0	P023	1 2 1 1 2	
7.297E+00	4.382E+02	5	D041	1 0 0 0 1	
5.088E+00	3.056E+02	7	J021	1 0 0 0 2	
5.246E+00	3.151E+02	10	D020	1 2 1 1 2	
5.246E+00	3.151E+02	10	D060	2 2 1 1 2	
7.651E+00	4.595E+02	10	M043	1 0 0 0 1	
7.602E+00	4.565E+02	10	P023	1 2 1 1 2	
5.550E+00	3.333E+02	17	J021	1 0 0 0 2	
7.382E+00	4.433E+02	18.72	S131	2 2 1 1 2	recrystallized
5.536E+00	3.324E+02	20	C052	1 2 1 1 2	
5.617E+00	3.373E+02	20	J021	1 0 0 0 2	
8.529E+00	5.122E+02	20	M043	1 0 0 0 2	
8.517E+00	5.115E+02	20	P023	1 2 1 1 2	
7.594E+00	4.561E+02	21.59	S131	2 2 1 1 2	recrystallized
7.738E+00	4.647E+02	23.85	S131	2 2 1 1 2	recrystallized
5.874E+00	3.528E+02	25	D020	1 2 1 1 2	
9.058E+00	5.440E+02	25	D041	1 0 0 0 2	
5.874E+00	3.528E+02	25	D060	2 2 1 1 2	
8.326E+00	5.000E+02	25	M136	2 0 0 0 2	
7.910E+00	4.750E+02	26.83	S131	2 2 1 1 2	recrystallized
7.966E+00	4.784E+02	27.31	S131	2 2 1 1 2	recrystallized
9.566E+00	5.745E+02	30	M043	1 0 0 0 2	
9.596E+00	5.763E+02	30	P023	1 2 1 1 2	
8.171E+00	4.907E+02	30.38	S131	2 2 1 1 2	recrystallized
6.244E+00	3.750E+02	35	J021	1 0 0 0 2	
1.712E+01	1.028E+03	35	S200	1 0 0 0 2	loc. cit.
8.469E+00	5.086E+02	35.15	S131	2 2 1 1 2	recrystallized
8.465E+00	5.083E+02	35.42	S131	2 2 1 1 2	recrystallized
8.575E+00	5.150E+02	37.36	S131	2 2 1 1 2	recrystallized
1.038E+01	6.232E+02	39.7	P023	1 2 1 1 2	
6.392E+00	3.839E+02	40	D020	1 2 1 1 2	
6.392E+00	3.839E+02	40	D060	2 2 1 1 2	
1.037E+01	6.226E+02	40	M043	1 0 0 0 2	
1.837E+01	1.103E+03	40	S200	1 0 0 0 2	loc. cit.
8.822E+00	5.298E+02	41.11	S131	2 2 1 1 2	recrystallized
8.982E+00	5.394E+02	43.85	S131	2 2 1 1 2	recrystallized
8.967E+00	5.386E+02	43.94	S131	2 2 1 1 2	recrystallized
1.961E+01	1.178E+03	45	S200	1 0 0 0 2	loc. cit.
9.107E+00	5.469E+02	46.56	S131	2 2 1 1 2	recrystallized
1.119E+01	6.721E+02	50	P023	1 2 1 1 2	

(*continued*)

22. CH_4N_2O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+01	1.267E+03	50	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.736E+02	50.6	P023	1 2 1 1 2	
9.560E+00	5.742E+02	54.77	S131	2 2 1 1 2	recrystallized
9.584E+00	5.756E+02	54.97	S131	2 2 1 1 2	recrystallized
2.283E+01	1.371E+03	55	S200	1 0 0 0 2	loc. cit.
9.649E+00	5.795E+02	55.88	S131	2 2 1 1 2	recrystallized
9.681E+00	5.814E+02	57.02	S131	2 2 1 1 2	recrystallized
9.806E+00	5.889E+02	59.13	S131	2 2 1 1 2	recrystallized
6.936E+00	4.166E+02	60	J021	1 0 0 0 2	
9.847E+00	5.914E+02	60	K013	1 0 1 1 2	
1.189E+01	7.143E+02	60	M043	1 0 0 0 2	
2.422E+01	1.455E+03	60	S200	1 0 0 0 2	loc. cit.
1.184E+01	7.110E+02	60.0	P023	1 2 1 1 2	
9.930E+00	5.963E+02	61.76	S131	2 2 1 1 2	recrystallized
1.005E+01	6.034E+02	63.79	S131	2 2 1 1 2	recrystallized
1.009E+01	6.060E+02	65	K013	1 0 1 1 2	
2.570E+01	1.543E+03	65	S200	1 0 0 0 2	loc. cit.
1.244E+01	7.468E+02	68.5	P023	1 2 1 1 2	
1.020E+01	6.127E+02	68.50	M059	1 1 2 1 2	
1.270E+01	7.629E+02	70	F300	1 0 0 0 2	
7.206E+00	4.328E+02	70	J021	1 0 0 0 2	
1.033E+01	6.206E+02	70	K013	1 0 1 1 2	
1.263E+01	7.588E+02	70	P023	1 2 1 1 2	
2.730E+01	1.640E+03	70	S200	1 0 0 0 2	loc. cit.
1.038E+01	6.231E+02	70.49	S131	2 2 1 1 2	recrystallized
1.048E+01	6.295E+02	73.11	S131	2 2 1 1 2	recrystallized
1.057E+01	6.345E+02	75	K013	1 0 1 1 2	
1.048E+01	6.296E+02	75.30	M059	1 1 2 1 2	
1.079E+01	6.480E+02	80	K013	1 0 1 1 2	
1.332E+01	8.000E+02	80	M043	1 0 0 0 2	
1.090E+01	6.546E+02	84.40	M059	1 1 2 1 2	
1.101E+01	6.610E+02	85	K013	1 0 1 1 2	
3.229E+01	1.939E+03	85	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.738E+02	90	K013	1 0 1 1 2	
3.426E+01	2.058E+03	90	S200	1 0 0 0 2	loc. cit.
1.131E+01	6.791E+02	93.80	M059	1 1 2 1 2	
1.142E+01	6.858E+02	95	K013	1 0 1 1 2	
3.611E+01	2.169E+03	95	S200	1 0 0 0 2	loc. cit.
1.161E+01	6.975E+02	100	K013	1 0 1 1 2	
1.465E+01	8.795E+02	100	M043	1 0 0 0 2	
3.778E+01	2.269E+03	100	S200	1 0 0 0 2	loc. cit.
1.177E+01	7.066E+02	104.40	M059	1 1 2 1 2	
1.199E+01	7.199E+02	109.90	M059	1 1 2 1 2	
1.219E+01	7.321E+02	115.30	M059	1 1 2 1 2	
1.229E+01	7.383E+02	118.30	M059	1 1 2 1 2	
1.234E+01	7.411E+02	118.70	M059	1 1 2 1 2	
1.245E+01	7.479E+02	121.90	M059	1 1 2 1 2	
1.249E+01	7.503E+02	123.20	M059	1 1 2 1 2	
1.264E+01	7.592E+02	127.50	M059	1 1 2 1 2	

(*continued*)

22. CH_4N_2O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E+01	7.619E+02	128.80	M059	1 1 2 1 2	
1.281E+01	7.694E+02	132.60	M059	1 1 2 1 2	
1.665E+01	1.000E+03	ns	B338	0 0 0 0 1	
1.332E+01	8.000E+02	ns	D072	0 0 0 0 0	

23. CH_4N_2S

Thiourea
Thiouree

RN: 62-56-6 **MP** (°C)**:** 176
MW: 76.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.136E-01	4.671E+01	0	M043	1 0 0 0 1	
9.731E-01	7.407E+01	10	M043	1 0 0 0 1	
1.118E+00	8.507E+01	10	O017	1 0 1 1 2	
1.206E+00	9.180E+01	13	F300	1 0 0 0 2	
1.206E+00	9.179E+01	13	O019	1 0 0 1 2	
1.383E+00	1.053E+02	15	O017	1 0 1 1 2	
1.573E+00	1.197E+02	20	M043	1 0 0 0 2	
1.544E+00	1.175E+02	20	O017	1 0 1 1 2	
1.085E+00	8.257E+01	25	I310	0 0 0 0 0	
1.759E+00	1.339E+02	25	O017	1 0 1 1 2	
2.199E+00	1.674E+02	30	M043	1 0 0 0 2	
3.093E+00	2.355E+02	40	M043	1 0 0 0 2	
5.455E+00	4.152E+02	60	M043	1 0 0 0 1	
7.617E+00	5.798E+02	80	M043	1 0 0 0 2	
9.250E+00	7.041E+02	100	M043	1 0 0 0 2	
7.882E-01	6.000E+01	ns	D072	0 0 0 0 0	

24. $CH_4N_4O_2$

α-Nitroguanidine
Nitroguanidine
Nitroguanidin

RN: 556-88-7 **MP** (°C)**:** 235
MW: 104.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.597E-02	2.703E+00	19.5	D027	1 2 0 0 2	
1.173E-01	1.221E+01	25	D022	1 1 2 2 2	
4.228E-02	4.400E+00	25	F300	1 0 0 0 1	
4.305E-02	4.480E+00	29.87	M028	1 2 2 1 0	EFG
1.122E-01	1.167E+01	50	D027	1 2 0 0 2	
3.070E-01	3.195E+01	71.67	M028	1 2 2 1 0	EFG
5.695E-01	5.927E+01	83.98	M028	1 2 2 1 0	EFG
9.025E-01	9.392E+01	100	D027	1 2 0 0 2	
7.620E-01	7.930E+01	100	F300	1 0 0 0 2	

25. CH_4O
Methanol
Methyl alcohol
RN: 67-56-1 **MP** (°C)**:** –97.8
MW: 32.04 **BP** (°C)**:** 64.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E+01	5.411E+02	ns	L003	0 0 2 1 2	

26. $CH_4O_6S_2$
Methionic acid
Acide methionique
Methanedisulfonic acid
RN: 503-40-2 **MP** (°C)**:** 98.0
MW: 176.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E+01	2.458E+03	25	B075	1 2 0 0 2	
4.035E+00	7.108E+02	25	B076	1 2 0 0 2	
4.862E+00	8.566E+02	25	F300	1 0 0 0 2	

27. $CH_4O_6S_2.H_2O$
Methionic acid (monohydrate)
RN: 503-40-2 MP (°C)**:**
MW: 194.18 BP (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.409E+00	8.562E+02	25	B076	1 2 0 0 2	

28. CH_5N
Methylamine
Aminomethane
Carbinamine
Mercurialin
RN: 74-89-5 **MP** (°C)**:** –93.5
MW: 31.06 **BP** (°C)**:** –6.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.906E+01	5.920E+02	4.50	F300	1 0 0 0 2	
2.963E+01	9.202E+02	12.5	D041	1 0 0 0 2	
2.147E+01	6.667E+02	12.50	M081	1 0 0 0 2	
1.916E+01	5.951E+02	20	M081	1 0 0 0 2	

(*continued*)

28. CH_5N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E+01	5.556E+02	25	M081	1 0 0 0 2	
1.664E+01	5.169E+02	30	M081	1 0 0 0 2	
1.380E+01	4.286E+02	40	M081	1 0 0 0 1	
1.143E+01	3.548E+02	50	M081	1 0 0 0 1	
9.034E+00	2.806E+02	60	M081	1 0 0 0 1	

29. $CH_5N_5O_2$
Nitroaminoguanidine
Hydrazinecarboximidamide, *N*-nitro-
1-Amino-3-nitroguanidine
3-Amino-1-nitroguanidine
1-Amino-2-nitroguanidine
1-Nitro-3-aminoguanidine
RN: 18264-75-0 **MP** (°C)**:** 185
MW: 119.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	1.619E+00	9.33	M047	2 2 1 1 0	EFG
2.254E-02	2.684E+00	20.96	M047	2 2 1 1 0	EFG
3.567E-02	4.248E+00	29.87	M047	2 2 1 1 0	EFG
4.384E-02	5.221E+00	34.53	M047	2 2 1 1 0	EFG
7.087E-02	8.440E+00	44.30	M047	2 2 1 1 0	EFG
9.318E-02	1.110E+01	49.42	M047	2 2 1 1 0	EFG

30. CH_5O_3As
Methanearsonic acid
MAA
Methylarsonsaeure
RN: 124-58-3 **MP** (°C)**:** 132
MW: 139.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E+00	2.038E+02	20	B200	1 0 0 0 2	
1.563E+00	2.188E+02	25	D305	1 0 0 0 1	

31. CH_5As
Methylarsine
Methylarsin
RN: 593-52-2 **MP** (°C)**:** –143
MW: 91.97 **BP** (°C)**:** 2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.242E-04	8.500E-02	20	F300	1 0 0 0 1	

32. $CBrClF_2$
Bromochlorodifluoromethane
Halon 1211
Chlorodifluorobromomethane
Bromochlorodifluoromethine
RN: 353-59-3 **MP** (°C)**:**
MW: 165.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.555E-05	1.580E-02	0	G055	1 2 2 2 1	

33. CBr_3F
Tribromo-fluoro-methane
Methane, tribromofluoro-
Fluorotribromomethane
RN: 353-54-8 **MP** (°C)**:**
MW: 270.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-03	3.998E-01	25	O006	1 0 0 0 1	

34. CBr_4
Carbon tetrabromide
Tetrabromomethane
RN: 558-13-4 **MP** (°C)**:** 89
MW: 331.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.235E-04	2.399E-01	30	G029	1 0 2 2 1	
6.998E-04	2.321E-01	30	V009	1 0 0 0 0	

35. CClN
Cyanogen chloride
Chlorcyan
RN: 506-77-4 **MP** (°C)**:** –6
MW: 61.47 **BP** (°C)**:** 13.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.761E-01	6.000E+01	0	F300	1 0 0 0 0	

36. $CClN_3O_6$
Chlorotrinitromethane
Chlor-trinitro-methan
RN: 1943-16-4 **MP** (°C)**:**
MW: 185.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.186E-02	2.200E+00	20	F300	1 0 0 0 1	

37. CCl_2F_2
Dichlorodifluoromethane
Difluorodichloromethane
Freon 12
RN: 75-71-8 **MP** (°C)**:** –158
MW: 120.91 **BP** (°C)**:** –29.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-02	1.867E+00	21	M065	1 0 2 1 2	
2.316E-03	2.800E–01	25	M133	1 0 0 0 2	
2.316E-03	2.800E–01	25	P046	1 0 0 0 0	
2.315E-03	2.799E–01	25	R048	0 0 0 0 0	

38. CCl_3F
Trichlorofluoromethane
Fluorotrichloromethane
Freon 11
RN: 75-69-4 **MP** (°C)**:** –111
MW: 137.37 **BP** (°C)**:** 23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.401E+00	20	H041	0 0 0 0 0	
8.008E-03	1.100E+00	20	M133	1 0 0 0 2	
8.008E-03	1.100E+00	20	P046	1 0 0 0 0	
1.020E-02	1.401E+00	21	H041	0 0 0 0 0	

(*continued*)

38. CCl_3F (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.013E-03	1.101E+00	25	H041	0 0 0 0 0	
7.999E-03	1.099E+00	25	R048	0 0 0 0 0	
7.997E-03	1.099E+00	27	H041	0 0 0 0 0	
7.853E-03	1.079E+00	30	H041	0 0 0 0 0	
9.892E-03	1.359E+00	31	H041	0 0 0 0 0	
4.152E-03	5.703E–01	50	H041	0 0 0 0 0	
2.258E-03	3.102E–01	75	H041	0 0 0 0 0	

39. CCl_3NO_2
Chloropicrin
Chlorpikrin
RN: 76-06-2 **MP** (°C)**:** –64
MW: 164.38 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.270E+00	0	M161	1 0 0 0 2	
1.396E-02	2.295E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
1.186E-02	1.950E+00	20	G080	1 0 0 0 1	
9.718E-03	1.597E+00	20	M061	1 0 0 0 1	
1.214E-02	1.996E+00	20	P081	1 0 0 0 0	
9.874E-03	1.623E+00	25	F300	1 0 0 0 2	
1.217E-02	2.000E+00	ns	N013	0 0 0 0 2	

40. CCl_4
Carbon tetrachloride
Tetrachloromethane
Methane tetrachloride
RN: 56-23-5 **MP** (°C)**:** –23
MW: 153.82 **BP** (°C)**:** 76.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.306E-03	9.700E-01	0	H101	2 0 0 0 1	
5.002E-03	7.694E-01	15	G029	1 0 2 2 1	
5.002E-03	7.694E-01	15	J036	0 0 0 0 0	
5.197E-03	7.994E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
5.201E-03	8.000E-01	20	H101	2 0 0 0 1	
5.201E-03	8.000E-01	20	M040	1 0 0 1 2	
5.103E-03	7.850E-01	20	M133	1 0 0 0 2	
5.200E-03	7.999E-01	20	M312	1 0 0 0 2	
4.612E-03	7.095E-01	20	N038	1 0 0 1 2	
5.103E-03	7.850E-01	20	P046	1 0 0 0 0	

(*continued*)

40. CCl_4 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.494E-03	9.990E-01	25	B019	1 0 1 2 0	
4.920E-03	7.568E-01	25	B173	2 0 2 2 2	
5.000E-03	7.691E-01	25	G038	1 2 2 2 1	
5.000E-03	7.691E-01	25	G053	2 1 2 1 1	
5.197E-03	7.994E-01	25	G056	1 0 0 0 2	
5.197E-03	7.994E-01	25	L319	1 0 2 1 1	
5.201E-03	8.000E-01	25	M037	1 1 0 0 0	
5.197E-03	7.994E-01	25	M061	1 0 0 0 0	
1.820E-03	2.800E-01	25	M161	1 0 0 0 1	
5.006E-03	7.700E-01	25	M368	1 0 0 0 1	
1.038E-02	1.597E+00	25	N034	1 0 0 0 1	*sic*
5.556E-03	8.546E-01	25	S133	1 1 1 1 1	
5.262E-03	8.093E-01	30	G029	1 0 2 2 1	
5.526E-03	8.500E-01	30	H101	2 0 0 0 1	
5.296E-03	8.146E-01	30	V009	1 0 0 0 1	
5.201E-03	8.000E-01	ns	F071	0 1 2 1 2	
5.201E-03	8.000E-01	ns	H080	0 0 0 0 2	
3.249E-03	4.998E-01	ns	I306	0 0 0 0 0	
5.201E-03	8.000E-01	ns	M344	0 0 0 0 2	

41. CF_4

Carbon tetrafluoride
Tetrafluoromethane

RN: 75-73-0 **MP** (°C)**:** –184
MW: 88.00 **BP** (°C)**:** –128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.319E-04	2.041E-02	19.99	C115	2 0 2 2 2	
2.083E-04	1.833E-02	24.99	C115	2 0 2 2 2	
2.111E-04	1.858E-02	25	D055	1 0 0 0 1	
1.940E-04	1.707E-02	29.99	C115	2 0 2 2 2	

42. COS

Carbonyl sulfide
Kohlenoxidsulfid

RN: 463-58-1 **MP** (°C)**:** –138
MW: 60.07 **BP** (°C)**:** –50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.259E-02	3.760E+00	0	F300	1 0 0 0 2	
2.081E-02	1.250E+00	25	F300	1 0 0 0 2	

43. CO_2

Carbon dioxide
Carbonic acid gas
Carbonic anhydride

RN: 124-38-9 **MP** (°C)**:** –57
MW: 44.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.641E-02	3.803E+00	16	B109	1 0 0 0 2	unit assumed, *sic*
8.377E-02	3.687E+00	17	B109	1 0 0 0 2	unit assumed, *sic*
8.641E-02	3.803E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
8.123E-02	3.575E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
7.886E-02	3.471E+00	19	B109	1 0 0 0 2	unit assumed, *sic*
7.654E-02	3.369E+00	20	B109	1 0 0 0 2	unit assumed, *sic*
7.432E-02	3.271E+00	21	B109	1 0 0 0 2	unit assumed, *sic*
7.427E-02	3.269E+00	21	B109	1 0 0 0 2	unit assumed, *sic*
7.213E-02	3.174E+00	22	B109	1 0 0 0 2	unit assumed, *sic*
6.582E-02	2.897E+00	25	B109	1 0 0 0 2	unit assumed, *sic*
3.360E-02	1.479E+00	25	H124	1 0 0 1 2	
6.204E-02	2.730E+00	27	B109	1 0 0 0 2	unit assumed, *sic*
6.127E-02	2.696E+00	28	B109	1 0 0 0 2	unit assumed, *sic*
5.714E-02	2.515E+00	30	B109	1 0 0 0 2	unit assumed, *sic*

44. CS_2

Carbon disulfide
Carbon disulphide
Schwefelkohlenstoff

RN: 75-15-0 **MP** (°C)**:** –112
MW: 76.14 **BP** (°C)**:** 46.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-02	2.040E+00	0	F300	1 0 0 0 2	
3.257E-02	2.480E+00	0	H101	2 0 0 0 2	
2.883E-02	2.195E+00	20	C121	0 0 0 0 1	unit assumed, *sic*
2.351E-02	1.790E+00	20	F300	1 0 0 0 2	
2.850E-02	2.170E+00	20	G080	1 0 0 0 1	
2.844E-02	2.165E+00	20	M061	1 0 0 0 2	
3.850E-02	2.931E+00	20	N038	1 0 0 1 2	
2.889E-02	2.200E+00	22	P076	1 2 1 1 1	
3.746E-02	2.852E+00	25	L319	1 0 2 1 1	
2.036E-02	1.550E+00	30	F300	1 0 0 0 2	
2.889E-02	2.200E+00	32	M161	1 0 0 0 1	
2.627E-02	2.000E+00	ns	N013	0 0 0 0 2	

45. $C_2HBrClF_3$

Halothane
2-Bromo-2-chloro-1,1,1-trifluoroethane
Fluothane

RN: 151-67-7 **MP** (°C)**:** <25
MW: 197.39 **BP** (°C)**:** 50.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-02	3.438E+00	ns	R028	0 0 0 0 0	

46. C_2HCl_3

Trichloroethylene
Trichloroethene
Trichloro-ethylene
Ethinyl trichloride
Acetylene trichloride
1,1,2-Trichloroethylene

RN: 79-01-6 **MP** (°C)**:** –87
MW: 131.39 **BP** (°C)**:** 86.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-03	1.100E+00	20	M133	1 0 0 0 2	
9.654E-03	1.268E+00	20	P041	1 0 0 0 1	
8.372E-03	1.100E+00	20	P046	1 0 0 0 0	
7.603E-03	9.990E–01	25	A094	1 0 0 0 1	
1.120E-02	1.472E+00	25	B173	2 0 2 2 2	
8.363E-03	1.099E+00	25	G056	1 0 0 0 2	
8.372E-03	1.100E+00	25	M037	1 1 0 0 1	
1.040E-02	1.366E+00	25	M342	1 0 1 1 2	
8.372E-03	1.100E+00	25	M368	1 0 0 0 1	
8.363E-03	1.099E+00	25	N034	1 0 0 0 1	
3.032E-02	3.984E+00	25	N309	1 0 0 0 1	*sic*
5.656E-03	7.431E–01	30	M311	1 1 2 2 2	
9.274E-03	1.219E+00	37	P041	1 0 0 0 1	
8.363E-03	1.099E+00	ns	O006	0 0 0 0 1	

47. $C_2HCl_3O.H_2O$

Chloral (monhydrate)
Chloral-hydrat

RN: 302-17-0 **MP** (°C)**:** 57.0
MW: 165.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E+00	3.400E+02	0	F300	1 0 0 0 2	
4.837E+00	8.000E+02	11.30	F300	1 0 0 0 2	
5.629E+00	9.310E+02	38.10	F300	1 0 0 0 2	
4.794E+00	7.930E+02	rt	D021	0 0 1 1 2	

48. $C_2HCl_3O_2$
Trichloroacetic acid
TCA
RN: 76-03-9 **MP** (°C)**:** 57.5
MW: 163.39 **BP** (°C)**:** 196.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.338E+00	5.455E+02	25	B185	0 0 0 0 0	
5.685E+00	9.289E+02	25	B200	1 0 0 0 2	
2.146E+00	3.506E+02	25	F018	1 0 0 0 1	
4.024E+00	6.575E+02	25	K040	1 2 1 2 2	
1.000E+01	1.634E+03	ns	M163	0 0 0 0 0	EFG
2.146E+00	3.506E+02	ns	N013	0 0 0 0 1	

49. C_2HCl_5
Pentachloroethane
Pentachloro-ethane
Pentalin
Pentachlorethane
Ethane pentachloride
RN: 76-01-7 **MP** (°C)**:** –29
MW: 202.30 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-03	4.698E-01	20	V009	1 0 0 0 1	
2.470E-03	4.998E-01	25	G056	1 0 0 0 2	
2.472E-03	5.000E-01	25	M037	1 1 0 0 1	
2.373E-03	4.800E-01	ns	H123	0 0 0 0 0	
2.322E-03	4.698E-01	ns	O006	0 0 0 0 1	

50. C_2H_2
Acetylene
Acetylen
RN: 74-86-2 **MP** (°C)**:** –81
MW: 26.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.796E-02	2.030E+00	0	F300	1 0 0 0 2	*sic*
4.609E-02	1.200E+00	20	F300	1 0 0 0 2	*sic*
1.862E+01	4.848E+02	25	M101	1 0 0 0 2	
1.959E-02	5.100E-01	60	F300	1 0 0 0 1	*sic*

51. $C_2H_2Br_4$

sym-Tetrabromoethane
1,1,2,2-Tetrabrom-aethan
Acetylene tetrabromide
1,1,2,2-Tetrabromoethane
Tetrabromoacetylene

RN: 79-27-6 **MP** (°C)**:** 0
MW: 345.67 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-03	6.500E-01	30	F300	1 0 0 0 1	
1.879E-03	6.496E-01	30	O006	1 0 0 0 1	

52. $C_2H_2Cl_2$

Vinylidene chloride
1,1-Dichloroethylene

RN: 75-35-4 **MP** (°C)**:** –122.0
MW: 96.94 **BP** (°C)**:** 31.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.470E–02	2.394E+00	15	D086	1 0 2 2 1	
2.624E-02	2.544E+00	17	D086	1 0 2 2 2	
4.126E-03	4.000E-01	20	M133	1 0 0 0 2	
4.126E-03	4.000E-01	20	P046	1 0 0 0 0	
2.572E-02	2.494E+00	20.5	D086	1 0 2 2 1	
2.316E-02	2.245E+00	25	D086	1 0 2 2 2	
2.470E-02	2.394E+00	28.5	D086	1 0 2 2 1	
2.624E-02	2.544E+00	29.5	D086	1 0 2 2 2	
2.302E-02	2.232E+00	30	M311	1 1 2 2 2	
2.264E-02	2.195E+00	38.5	D086	1 0 2 2 1	
2.162E-02	2.096E+00	45	D086	1 0 2 2 1	
2.367E-02	2.295E+00	51	D086	1 0 2 2 1	
2.162E-02	2.096E+00	55	D086	1 0 2 2 1	
2.470E-02	2.394E+00	60	D086	1 0 2 2 1	
2.316E-02	2.245E+00	65	D086	1 0 2 2 2	
3.034E-02	2.941E+00	71	D086	1 0 2 2 2	
2.572E-02	2.494E+00	74.5	D086	1 0 2 2 1	
3.034E-02	2.941E+00	81	D086	1 0 2 2 2	
3.803E-02	3.686E+00	85.5	D086	1 0 2 2 1	
3.598E-02	3.488E+00	90.5	D086	1 0 2 2 1	

53. $C_2H_2Cl_2$
cis-Acetylene dichloride
cis-1,2-Dichloroethylene
cis-Dichlorethylene
RN: 156-59-2 **MP** (°C)**:** –80
MW: 96.94 **BP** (°C)**:** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E-02	3.500E+00	25	M037	1 1 0 0 1	

54. $C_2H_2Cl_2$
trans-Acetylene dichloride
trans-1,2-Dichloroethylene
trans-Dichlorethylene
RN: 156-60-5 **MP** (°C)**:** –50
MW: 96.94 **BP** (°C)**:** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.499E-02	6.300E+00	25	M037	1 1 0 0 1	

55. $C_2H_2Cl_3As$
Chlorovinyldichloroarsine
Chlorvinylarsin-dichlorid
RN: 541-25-3 **MP** (°C)**:**
MW: 207.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-03	5.000E-01	20	F300	1 0 0 0 0	

56. $C_2H_2Cl_4$
1,1,1,2-Tetrachloroethane
Ethane, 1,1,1,2-tetrachloro-
F 130α
TCA
HCC 130α
RN: 630-20-6 **MP** (°C)**:** –44
MW: 167.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.141E-03	1.199E+00	0	V009	1 0 0 0 2	
6.487E-03	1.089E+00	20	V009	1 0 0 0 2	
1.723E-02	2.892E+00	25	G056	1 0 0 0 2	
<1.66E-02	<2.79E+00	25.50	O005	2 0 2 2 1	
6.843E-03	1.149E+00	35	V009	1 0 0 0 2	
7.438E-03	1.248E+00	50	V009	1 0 0 0 2	

57. $C_2H_2Cl_4$
1,1,2,2-Tetrachloroethane
sym-Tetrachloroethane
RN: 79-34-5 **MP** (°C)**:** –36
MW: 167.85 **BP** (°C)**:** 146.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.924E-02	3.230E+00	20	C094	1 0 0 0 2	
1.758E-02	2.951E+00	23.5	S171	2 1 2 2 2	
1.770E-02	2.971E+00	25	B173	2 0 2 2 2	
1.782E-02	2.991E+00	25	F050	1 0 0 0 0	
1.728E-02	2.900E+00	25	M037	1 1 0 0 1	
1.737E-02	2.915E+00	30	M311	1 1 2 2 2	

58. $C_2H_2O_4$
Oxalic acid
Oxalsaeure
RN: 144-62-7 **MP** (°C)**:** 189
MW: 90.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.683E-01	3.316E+01	0	C066	1 0 1 1 2	
3.665E-01	3.300E+01	0	L041	1 0 0 1 1	
3.756E-01	3.382E+01	0	M043	1 0 0 0 1	
4.907E-01	4.418E+01	4.99	A339	0 0 0 0 0	
6.287E-01	5.660E+01	10	M043	1 0 0 0 1	
5.912E-01	5.323E+01	9.99	A339	0 0 0 0 0	
7.752E-01	6.979E+01	14.99	A339	0 0 0 0 0	
7.441E-01	6.700E+01	15	F066	2 2 2 2 1	
7.464E-01	6.720E+01	15	F300	1 0 0 0 2	
7.775E-01	7.000E+01	15	L041	1 0 0 1 1	
9.468E-01	8.524E+01	19.99	A339	0 0 0 0 0	
9.219E-01	8.300E+01	20	F066	2 2 2 2 1	
9.219E-01	8.300E+01	20	F300	1 0 0 0 1	
9.552E-01	8.600E+01	20	L041	1 0 0 1 1	
9.636E-01	8.676E+01	20	M043	1 0 0 0 1	
8.836E-01	7.956E+01	20	M171	1 0 0 0 1	
1.146E+00	1.032E+02	24.99	A339	0 0 0 0 0	
1.088E+00	9.800E+01	25	F066	2 2 2 2 1	
1.378E+00	1.240E+02	25	F317	2 1 1 1 2	
2.480E+00	2.233E+02	25	H084	1 0 0 0 2	
1.190E+00	1.071E+02	25	H430	0 0 0 0 0	
2.409E+00	2.169E+02	25	K040	1 0 2 1 2	
1.317E+00	1.186E+02	29.99	A339	0 0 0 0 0	
1.407E+00	1.266E+02	30	M043	1 0 0 0 2	
1.623E+00	1.461E+02	34.99	A339	0 0 0 0 0	
1.710E+00	1.540E+02	35	L041	1 0 0 1 2	
1.903E+00	1.713E+02	39.99	A339	0 0 0 0 0	

(*continued*)

58. $C_2H_2O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.973E+00	1.776E+02	40	M043	1 0 0 0 2	
2.199E+00	1.979E+02	44.99	A339	0 0 0 0 0	
2.527E+00	2.275E+02	49.99	A339	0 0 0 0 0	
2.150E+00	1.935E+02	50	C066	1 0 1 1 2	
2.821E+00	2.540E+02	50	L041	1 0 0 1 2	
2.867E+00	2.581E+02	54.99	A339	0 0 0 0 0	
3.121E+00	2.810E+02	59.99	A339	0 0 0 0 0	
3.410E+00	3.070E+02	60	M043	1 0 0 0 2	
3.661E+00	3.296E+02	64.99	A339	0 0 0 0 0	
4.121E+00	3.710E+02	65	L041	1 0 0 1 2	
3.583E+00	3.226E+02	80	C066	1 0 1 1 2	
5.084E+00	4.577E+02	80	M043	1 0 0 0 2	
6.059E+00	5.455E+02	90	F300	1 0 0 0 2	

59. $C_2H_2O_4.2H_2O$
Oxalic acid dihydrate
Ethanedioic acid, dihydrate
RN: 6153-56-6 **MP** (°C)**:** 101
MW: 126.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-02	1.820E+00	23	C038	2 2 2 2 0	EFG, 0.1N HCl
1.070E-02	1.349E+00	30	C038	2 2 2 2 0	EFG, 0.1N HCl
7.234E-03	9.120E-01	35	C038	2 2 2 2 0	EFG, 0.1N HCl

60. $C_2H_3Br_3O$
2,2,2-Tribromoethanol
2,2,2-Tribrom-aethanol
RN: 75-80-9 **MP** (°C)**:** 80
MW: 282.77 **BP** (°C)**:** 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-01	3.410E+01	40	F300	1 0 0 0 2	

61. C_2H_3Cl

Vinyl chloride
Chloroethylene

RN: 75-01-4 **MP** (°C)**:** –153.0
MW: 62.50 **BP** (°C)**:** –13.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	6.000E-02	10	M133	1 0 0 0 1	*sic*
9.600E-04	6.000E-02	10	P046	1 0 0 0 0	*sic*
1.506E-01	9.411E+00	15	D086	1 0 2 2 1	
1.576E-01	9.852E+00	16	D086	1 0 2 2 2	
1.081E-01	6.754E+00	20	N034	1 0 0 0 1	
1.451E-01	9.067E+00	20.5	D086	1 0 2 2 2	
<1.76E-02	<1.10E+00	25	I310	0 0 0 0 0	
1.396E-01	8.723E+00	26	D086	1 0 2 2 1	
1.411E-01	8.821E+00	29.5	D086	1 0 2 2 1	
1.490E-01	9.312E+00	35	D086	1 0 2 2 1	
1.411E-01	8.821E+00	41	D086	1 0 2 2 1	
1.396E-01	8.723E+00	46.5	D086	1 0 2 2 1	
6.717E-03	4.198E-01	50	M065	0 0 2 1 1	
1.506E-01	9.411E+00	55	D086	1 0 2 2 1	
1.459E-01	9.116E+00	65	D086	1 0 2 2 1	
1.553E-01	9.705E+00	72.5	D086	1 0 2 2 1	
1.584E-01	9.901E+00	80	D086	1 0 2 2 2	
1.772E-01	1.108E+01	85	D086	1 0 2 2 2	

62. $C_2H_3Cl_2NO_2$

1,1-Dichloro-1-nitroethane
Dichloronitroethane
Ethide

RN: 594-72-9 **MP** (°C)**:**
MW: 143.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.456E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
1.732E-02	2.494E+00	20	M061	1 0 0 0 1	

63. $C_2H_3Cl_3$
1,1,1-Trichloroethane
1,1,1-Trichloroethane
Trichloroethane
1,1,1-Trichloethane
RN: 71-55-6 **MP** (°C)**:** –35
MW: 133.41 **BP** (°C)**:** 74.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-02	1.587E+00	0	V009	1 0 0 0 2	
1.342E-02	1.790E+00	3.5	C094	1 0 0 0 2	
1.019E-02	1.360E+00	20	C094	1 0 1 0 2	
3.358E-02	4.480E+00	20	G056	1 0 0 0 2	
3.598E-03	4.800E-01	20	M133	1 0 0 0 2	
9.895E-03	1.320E+00	20	M368	1 0 0 0 1	
3.598E-03	4.800E-01	20	P046	1 0 0 0 0	
9.882E-03	1.318E+00	20	V009	1 0 0 0 2	
8.797E-03	1.174E+00	23.5	S171	2 1 2 2 2	
5.244E-03	6.995E-01	25	A094	1 0 0 0 0	
1.000E-02	1.334E+00	25	B173	2 0 2 2 2	
3.284E-02	4.381E+00	25	N309	1 0 0 0 1	*sic*
9.732E-03	1.298E+00	25	O006	1 0 0 0 1	
3.597E-03	4.798E-01	30	M311	1 1 2 2 2	
9.433E-03	1.258E+00	35	V009	1 0 0 0 2	
9.583E-03	1.278E+00	50	V009	1 0 0 0 2	
5.397E-03	7.200E-01	ns	H123	0 0 0 0 0	

64. $C_2H_3Cl_3$
1,1,2-Trichloroethane
1,1,2-β-Trichloroethane
RN: 79-00-5 **MP** (°C)**:** –37
MW: 133.41 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-02	4.638E+00	0	V009	1 0 0 0 2	
3.254E-02	4.341E+00	20	V009	1 0 0 0 2	
3.804E-02	5.074E+00	25	C119	2 2 2 2 2	
3.298E-02	4.400E+00	25	M037	1 1 0 0 1	
3.272E-02	4.365E+00	30	M311	1 1 2 2 2	
3.417E-02	4.559E+00	35	V009	1 0 0 0 2	
3.967E-02	5.292E+00	55	V009	1 0 0 0 2	

65. $C_2H_3FO_2$
Fluoroacetic acid
Essigsaeurefluorid
RN: 144-49-0 **MP** (°C)**:**
MW: 78.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.407E-04	5.000E-02	20	F300	1 0 0 0 0	

66. C_2H_3N
Acetonitrile
Acetonitril
RN: 75-05-8 **MP** (°C)**:** –45
MW: 41.05 **BP** (°C)**:** 81.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.95E+01	>8.00E+02	25	B019	1 0 1 2 0	

67. C_2H_3N
Methylisocyanide
Methyl-isocyanid
RN: 593-75-9 **MP** (°C)**:**
MW: 41.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E+00	9.100E+01	15	F300	1 0 0 0 1	

68. C_2H_3NS
Methyl isothiocyanate
Isothiocyanatomethane
RN: 556-61-6 **MP** (°C)**:** 35
MW: 73.12 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	7.600E+00	20	M161	1 0 0 0 1	
1.032E-01	7.543E+00	20	O300	1 0 0 0 1	
1.085E-01	7.937E+00	20	P081	1 0 0 0 0	

69. C_2H_4
Ethylene
Ethene
RN: 74-85-1 **MP** (°C)**:** –169
MW: 28.05 **BP** (°C)**:** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E+00	2.000E+02	0	R028	0 0 0 0 0	
3.240E+00	9.091E+01	25	R028	0 0 0 0 0	
3.187E+00	8.942E+01	30	C116	0 0 0 0 0	

70. C_2H_4BrCl
Ethylene chlorobromide
1-Bromo-2-chloroethane
RN: 107-04-0 **MP** (°C)**:** –17
MW: 143.42 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.778E-02	6.853E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

71. $C_2H_4Br_2$
1,2-Dibromoethane
Ethylene dibromide
Curafume
Haltox
1,2-Dibromaethan
RN: 106-93-4 **MP** (°C)**:** 9.97
MW: 187.87 **BP** (°C)**:** 131.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.777E-02	3.339E+00	0	V009	1 0 0 0 2	
2.078E-02	3.905E+00	15	G029	1 0 2 2 2	
1.874E-02	3.520E+00	20	C094	1 0 1 0 2	
2.279E-02	4.282E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
1.794E-02	3.370E+00	20	G080	1 0 0 0 1	
2.300E-02	4.321E+00	20	M312	1 0 0 0 1	
1.592E-02	2.991E+00	20	P081	1 0 0 0 0	
2.142E-02	4.024E+00	20	V009	1 0 0 0 2	
2.210E-02	4.153E+00	25	O006	1 0 0 0 2	
2.294E-02	4.310E+00	30	F300	1 0 0 0 2	
2.284E-02	4.292E+00	30	G029	1 0 2 2 2	
2.279E-02	4.282E+00	30	M061	1 0 0 0 1	
2.289E-02	4.300E+00	30	M161	1 0 0 0 1	
2.390E-02	4.490E+00	35	V009	1 0 0 0 2	
2.817E-02	5.292E+00	50	V009	1 0 0 0 2	

72. C_2H_4ClNO

Acetohydroxamic acid chloride
Acethydroximsaeure-chlorid
2-Chloroacetamide
Chloroacetamide
Chloressigsaeureamid
Essigsaeure-*N*-chloramid

RN: 79-07-2 **MP** (°C)**:** 119.5
MW: 93.51 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.624E-01	9.000E+01	24	F300	1 0 0 0 0	

73. $C_2H_4ClNO_2$

1-Chloro-1-nitroethane
1-Chloronitroethane

RN: 598-92-5 **MP** (°C)**:**
MW: 109.51 **BP** (°C)**:** 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.638E-02	3.984E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
3.638E-02	3.984E+00	20	M061	1 0 0 0 0	

74. $C_2H_4Cl_2$

Ethylidene chloride
1,1-Dichloraethan
1,1-Dichloroethane

RN: 75-34-3 **MP** (°C)**:** –97
MW: 98.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-02	6.600E+00	0	F300	1 0 0 0 1	
6.629E-02	6.560E+00	0	H101	2 0 0 0 2	
5.967E-02	5.905E+00	0	V009	1 0 0 0 2	
5.558E-02	5.500E+00	20	F300	1 0 0 0 1	
5.558E-02	5.500E+00	20	H101	2 0 0 0 2	
5.087E-02	5.035E+00	20	V009	1 0 0 0 2	
5.110E-02	5.057E+00	25	G038	1 2 2 2 2	
5.110E-02	5.057E+00	25	G053	2 2 2 1 2	
5.457E-02	5.400E+00	30	F300	1 0 0 0 1	
4.885E-02	4.834E+00	30	M300	1 1 2 2 2	
4.637E-02	4.589E+00	30	M311	1 1 2 2 2	
5.397E-02	5.341E+00	30	N034	1 0 0 0 2	
4.847E-02	4.797E+00	35	V009	1 0 0 0 2	
5.217E-02	5.163E+00	50	V009	1 0 0 0 2	

75. $C_2H_4Cl_2$

Ethylene dichloride
1,2-Dichloraethan

RN: 107-06-2 **MP** (°C)**:** –35
MW: 98.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.095E-02	9.000E+00	0	F300	1 0 0 0 0	
9.317E-02	9.220E+00	0	H101	2 0 0 0 2	
9.232E-02	9.136E+00	0	L103	1 0 0 0 2	unit assumed
8.745E-02	8.654E+00	0	V009	1 0 0 0 2	
8.735E-02	8.645E+00	15	G029	1 0 2 2 2	
8.539E-02	8.450E+00	20	C094	1 0 1 0 2	
8.716E-02	8.625E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
8.716E-02	8.625E+00	20	D052	1 1 0 0 1	
8.716E-02	8.625E+00	20	G056	1 0 0 0 2	
8.781E-02	8.690E+00	20	H101	2 0 0 0 2	
8.706E-02	8.615E+00	20	L103	1 0 0 0 2	unit assumed
8.706E-02	8.615E+00	20	M061	1 0 0 0 2	
8.616E-02	8.527E+00	20	M062	1 0 0 0 1	
8.892E-02	8.800E+00	20	M133	1 0 0 0 2	
8.716E-02	8.625E+00	20	O006	1 0 0 0 1	
8.892E-02	8.800E+00	20	P046	1 0 0 0 0	
8.507E-02	8.419E+00	20	V009	1 0 0 0 2	
8.070E-02	7.986E+00	25	B173	2 0 2 2 2	
1.060E-01	1.049E+01	25	C119	2 2 2 2 2	
8.690E-02	8.600E+00	25	F300	1 0 0 0 2	
8.740E-02	8.649E+00	25	G038	1 2 2 2 2	
8.740E-02	8.649E+00	25	G053	2 1 2 1 2	
8.488E-02	8.400E+00	25	M037	1 1 0 0 1	
9.013E-02	8.920E+00	30	G029	1 0 2 2 1	
8.954E-02	8.861E+00	30	L103	1 0 0 0 2	unit assumed
3.543E-02	3.506E+00	30	M311	1 1 2 2 2	
8.964E-02	8.871E+00	35	V009	1 0 0 0 2	
1.030E-01	1.019E+01	56	V009	1 0 0 0 2	
8.716E-02	8.625E+00	72	B197	0 0 0 0 0	at bp of 72 °C
5.927E-02	5.865E+00	89.3	B197	0 0 0 0 0	at bp of 89.3 °C
4.327E-02	4.282E+00	92.3	B197	0 0 0 0 0	at bp of 92.3 °C
3.324E-02	3.289E+00	94	B197	0 0 0 0 0	at bp of 94 °C
1.312E-02	1.298E+00	98	B197	0 0 0 0 0	at bp of 98 °C
4.345E-02	4.300E+00	rt	M161	0 0 0 0 1	

76. $C_2H_4F_2$

1,1-Difluoroethane
Ethylidene fluoride

RN: 75-37-6 **MP** (°C)**:** –117
MW: 66.05 **BP** (°C)**:** –24.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.132E-02	5.371E+00	0	M065	0 0 2 1 2	

77. $C_2H_4N_2O_2$
Oxamide
Oxalsaeure-diamid
RN: 471-46-5 **MP** (°C)**:**
MW: 88.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-03	3.700E-01	7.30	F300	1 0 0 0 1	
7.040E-02	6.200E+00	100	F300	1 0 0 0 1	

78. $C_2H_4N_4$
Amitrole
3-Amino-1,2,4-triazole
3-Amino-*s*-triazole
ATA
Aminotriazole
RN: 61-82-5 **MP** (°C)**:** 159.0
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	2.188E+02	23	M061	1 0 0 0 1	
2.602E+00	2.188E+02	25	B185	0 0 0 0 0	
2.602E+00	2.188E+02	25	B200	1 0 0 0 1	
2.602E+00	2.188E+02	25	I310	0 0 0 0 0	
3.330E+00	2.800E+02	25	M161	1 0 0 0 2	
2.602E+00	2.188E+02	ns	B100	0 0 0 0 1	
3.162E+00	2.659E+02	ns	M163	0 0 0 0 0	EFG

79. $C_2H_4N_4$
Dicyanodiamide
Dicyandiamid
Dicyandiamide
RN: 461-58-5 **MP** (°C)**:** 210
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E-01	1.283E+01	0	M043	1 0 0 0 1	
2.218E-01	1.865E+01	10	M043	1 0 0 0 1	
2.617E-01	2.200E+01	13	F300	1 0 0 0 1	
3.688E-01	3.101E+01	20	M043	1 0 0 0 1	
4.876E-01	4.100E+01	25	F300	1 0 0 0 1	
4.717E-01	3.966E+01	25.0	H037	1 2 2 1 2	
5.663E-01	4.762E+01	30	M043	1 0 0 0 1	
8.565E-01	7.201E+01	39.9	H037	1 2 2 1 2	
8.606E-01	7.236E+01	40	M043	1 0 0 0 1	
1.255E+00	1.055E+02	49.8	H037	1 2 2 1 2	

(*continued*)

79. $C_2H_4N_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.899E+00	1.597E+02	60	M043	1 0 0 0 1	
1.878E+00	1.579E+02	60.1	H037	1 2 2 1 2	
2.236E+00	1.880E+02	60.10	F300	1 0 0 0 2	
2.978E+00	2.504E+02	74.5	H037	1 2 2 1 2	
3.275E+00	2.754E+02	80	M043	1 0 0 0 1	
1.492E-01	1.254E+01	.0	H037	1 2 2 1 2	

80. $C_2H_4N_4O_2S_2$
2-Amino-1,3,4-thiadiazole-5-sulfonamide
5-Amino-1,3,4-thiadiazol-2-sulfonamide
5-Amino-1,3,4-thiadiazole-2-sulfonamide
CL 5343
Tio-urasin
RN: 14949-00-9 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-02	4.739E+00	15	K024	1 2 1 1 2	

81. $C_2H_4O_2$
Acetic acid glacial
Acetic acid
Essigsaeure
RN: 64-19-7 **MP** (°C)**:** 16.7
MW: 60.05 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E+01	6.029E+02	25	H084	1 0 0 0 2	

82. $C_2H_4O_2$
Methyl formate
Methyl methanoate
Formic acid methyl ester
RN: 107-31-3 **MP** (°C)**:** –99.8
MW: 60.05 **BP** (°C)**:** 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.80E+00	+2.28E+02	ns	S460	0 0 0 0 0	

83. $C_2H_4O_3$
Glycolic acid
Glykolsaeure
RN: 79-14-1 **MP** (°C)**:** 80
MW: 76.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.084E+00	4.627E+02	6.99	A340	0 0 0 0 0	
6.913E+00	5.258E+02	10.89	A340	0 0 0 0 0	
7.894E+00	6.004E+02	20.69	A340	0 0 0 0 0	
8.015E+00	6.096E+02	24.99	A340	0 0 0 0 0	
8.168E+00	6.212E+02	30.09	A340	0 0 0 0 0	
8.296E+00	6.309E+02	35.99	A340	0 0 0 0 0	
8.400E+00	6.388E+02	39.99	A340	0 0 0 0 0	
8.533E+00	6.489E+02	47.99	A340	0 0 0 0 0	
8.536E+00	6.492E+02	48.99	A340	0 0 0 0 0	
8.654E+00	6.582E+02	54.99	A340	0 0 0 0 0	
8.721E+00	6.632E+02	59.49	A340	0 0 0 0 0	
8.808E+00	6.698E+02	64.49	A340	0 0 0 0 0	
8.866E+00	6.743E+02	69.99	A340	0 0 0 0 0	
8.932E+00	6.793E+02	74.99	A340	0 0 0 0 0	
8.968E+00	6.820E+02	79.89	A340	0 0 0 0 0	
9.016E+00	6.857E+02	84.49	A340	0 0 0 0 0	
9.043E+00	6.877E+02	88.09	A340	0 0 0 0 0	

84. C_2H_5Br
Bromoethane
Ethyl bromide
Aethylbromid
RN: 74-96-4 **MP** (°C)**:** –119
MW: 108.97 **BP** (°C)**:** 38.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.792E-02	1.067E+01	0	H101	2 0 0 0 2	
8.810E-02	9.600E+00	17.5	F001	1 0 1 2 2	
8.810E-02	9.600E+00	17.5	S006	1 0 0 0 2	
8.259E-02	9.000E+00	20	F300	1 0 0 0 0	
8.388E-02	9.140E+00	20	H101	2 0 0 0 2	
8.185E-02	8.920E+00	20	H127	1 0 0 0 0	
8.127E-02	8.856E+00	30	V009	1 0 0 0 1	

85. C_2H_5Cl
Ethyl chloride
Aethylchlorid
Chloroethane
Monochloroethane
RN: 75-00-3 **MP** (°C)**:** –139.0
MW: 64.52 **BP** (°C)**:** 12.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-02	4.500E+00	0	M037	1 1 0 0 1	
6.898E-02	4.450E+00	0	V009	1 0 0 0 2	
7.865E-02	5.074E+00	20	G056	1 0 0 0 2	
8.846E-02	5.707E+00	20	N034	1 0 0 0 2	
8.900E-02	5.742E+00	ns	F001	0 0 1 2 2	
8.433E-02	5.440E+00	ns	R028	0 0 0 0 0	

86. C_2H_5I
Iodoethane
Ethyl iodide
Aethyliodid
Iodaethan
RN: 75-03-6 **MP** (°C)**:** –108
MW: 155.97 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-02	4.410E+00	0	H101	2 0 0 0 2	
2.571E-02	4.010E+00	20	F300	1 0 0 0 2	
2.584E-02	4.030E+00	20	H101	2 0 0 0 2	
2.510E-02	3.915E+00	20	M171	1 0 0 0 2	
2.510E-02	3.915E+00	22.5	F001	1 0 1 2 2	
2.510E-02	3.915E+00	22.5	S006	1 0 0 0 2	
2.580E-02	4.024E+00	30	G029	1 0 2 2 2	
2.661E-02	4.150E+00	30	H101	2 0 0 0 2	
2.580E-02	4.023E+00	30	V009	1 0 0 0 2	

87. C_2H_5N
Ethylenimine
Aethylenimin
Aziridine
Ethyleneimine
Dimethyleneimine
RN: 151-56-4 **MP** (°C)**:** –78
MW: 43.07 **BP** (°C)**:** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.117E-01	9.116E+00	20	P315	0 0 0 0 0	

88. C_2H_5NO
Acetamide
Acetamid
RN: 60-35-5 **MP** (°C)**:** 81.0
MW: 59.07 **BP** (°C)**:** 222.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E+01	6.030E+02	.3	F300	1 0 0 0 2	
8.342E+00	4.927E+02	0	M022	1 0 0 0 2	
9.816E+00	5.798E+02	0	M043	1 0 0 0 2	
1.077E+01	6.364E+02	10	M043	1 0 0 0 2	
1.165E+01	6.880E+02	20	F300	1 0 0 0 2	
9.691E+00	5.724E+02	20	M022	1 0 0 0 2	
1.180E+01	6.970E+02	20	M043	1 0 0 0 2	
1.194E+01	7.050E+02	24.50	F300	1 0 0 0 2	
3.386E+01	2.000E+03	25	I310	0 0 0 0 0	
1.280E+01	7.561E+02	30	M043	1 0 0 0 2	
1.093E+01	6.455E+02	40	M022	1 0 0 0 2	
1.379E+01	8.148E+02	40	M043	1 0 0 0 2	
1.208E+01	7.138E+02	60	M022	1 0 0 0 2	
1.515E+01	8.947E+02	60	M043	1 0 0 0 2	
8.358E+00	4.937E+02	rt	D021	0 0 1 1 2	

89. $C_2H_5NO_2$
Glycine
Glycin
Glycocoll
RN: 56-40-6 **MP** (°C)**:** 245
MW: 75.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E+00	1.252E+02	0	D018	2 2 2 1 2	
1.656E+00	1.243E+02	0	M043	1 0 0 0 2	
1.905E+00	1.430E+02	10	C347	0 0 0 0 0	EFG
2.032E+00	1.525E+02	10	M043	1 0 0 0 2	
3.025E+00	2.271E+02	15	D349	2 1 1 2 2	
1.710E+00	1.284E+02	15	G081	1 0 1 1 2	
3.009E+00	2.259E+02	20	B032	1 2 2 2 2	
2.336E+00	1.754E+02	20	C347	0 0 0 0 0	EFG
3.180E+00	2.387E+02	20	D349	2 1 1 2 2	
2.447E+00	1.837E+02	20	M043	1 0 0 0 2	
2.616E+00	1.964E+02	21	P045	1 0 2 1 2	
2.127E+00	1.597E+02	22.9	Y412	0 0 0 0 0	
2.741E+00	2.058E+02	24.99	C404	2 1 2 2 1	
3.316E+00	2.489E+02	25	B032	1 2 2 2 2	
2.885E+00	2.166E+02	25	C018	0 0 0 0 0	
2.700E-03	2.027E-01	25	C405	2 1 2 2 2	intrinsic zwit

(*continued*)

89. $C_2H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.329E+00	2.499E+02	25	D016	1 0 0 0 2	
2.691E+00	2.020E+02	25	D018	2 2 2 1 2	
2.663E+00	1.999E+02	25	D041	1 0 0 0 2	
3.325E+00	2.496E+02	25	D349	2 1 1 2 2	
2.886E+00	2.166E+02	25	E015	1 2 1 1 2	
2.660E+00	1.997E+02	25	F300	1 0 0 0 2	
2.664E+00	2.000E+02	25	G092	2 1 1 1 1	
2.664E+00	2.000E+02	25	G315	0 0 0 0 0	
2.526E+00	1.897E+02	25	K031	2 1 2 1 2	
2.886E+00	2.166E+02	25	M024	1 2 0 1 2	
3.334E+00	2.503E+02	25	M029	2 2 2 2 2	
2.760E+00	2.072E+02	25	N001	0 0 0 0 0	EFG
2.900E+00	2.177E+02	25	N012	2 0 2 1 2	
2.544E+00	1.910E+02	25	O316	1 0 1 2 2	
2.664E+00	2.000E+02	25	O316	1 0 1 2 2	
2.715E+00	2.038E+02	25	O317	1 0 1 2 2	
3.330E+00	2.500E+02	25.1	N024	0 0 0 0 0	
3.352E+00	2.516E+02	25.1	N025	0 0 0 0 0	
3.342E+00	2.509E+02	25.1	N026	0 0 0 0 0	
2.673E+00	2.006E+02	25.1	N027	1 1 2 2 2	
2.220E+00	1.667E+02	25.3	Y412	0 0 0 0 0	
3.144E+00	2.360E+02	27	D036	0 0 0 0 0	
3.074E+00	2.308E+02	27	D036	0 0 0 0 0	
2.312E+00	1.736E+02	29.2	Y412	0 0 0 0 0	
3.630E+00	2.725E+02	29.80	B032	1 2 2 1 2	
2.737E+00	2.054E+02	30	C347	0 0 0 0 0	EFG
2.832E+00	2.126E+02	30	M043	1 0 0 0 1	
3.106E+00	2.332E+02	34.99	C404	2 1 2 2 1	
2.491E+00	1.870E+02	36.8	Y412	0 0 0 0 0	
2.578E+00	1.935E+02	38.2	Y412	0 0 0 0 0	
3.109E+00	2.334E+02	40	C347	0 0 0 0 0	EFG
3.305E+00	2.481E+02	40	M043	1 0 0 0 1	
3.538E+00	2.656E+02	44.99	C404	2 1 2 2 1	
2.749E+00	2.063E+02	45.5	Y412	0 0 0 0 0	
3.547E+00	2.662E+02	50	C347	0 0 0 0 0	EFG
3.816E+00	2.865E+02	50	D018	2 2 2 1 2	
3.745E+00	2.811E+02	50	F300	1 0 0 0 2	
3.921E+00	2.943E+02	60	C347	0 0 0 0 0	EFG
4.134E+00	3.103E+02	60	M043	1 0 0 0 1	
4.215E+00	3.164E+02	70	C347	0 0 0 0 0	EFG
4.863E+00	3.650E+02	75	D018	2 2 2 1 2	
4.693E+00	3.523E+02	75	D041	1 0 0 0 2	
4.693E+00	3.523E+02	75	F300	1 0 0 0 2	
4.517E+00	3.390E+02	80	C347	0 0 0 0 0	EFG
4.836E+00	3.631E+02	80	M043	1 0 0 0 1	
4.753E+00	3.568E+02	90	C347	0 0 0 0 0	EFG
4.911E+00	3.686E+02	100	C347	0 0 0 0 0	EFG
5.353E+00	4.018E+02	100	F300	1 0 0 0 2	

(*continued*)

89. $C_2H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.485E+00	4.118E+02	100	M043	1 0 0 0 1	
5.353E+00	4.018E+02	99.99	P349	0 0 0 0 0	
1.612E+00	1.210E+02	—	C347	0 0 0 0 0	EFG
6.661E+00	5.000E+02	ns	D072	0 0 0 0 0	
4.499E+00	3.377E+02	rt	D021	0 0 1 1 2	

90. $C_2H_5NO_2$
Nitroethane
Nitroetan
RN: 79-24-3 **MP** (°C)**:** –50
MW: 75.07 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.736E-01	4.306E+01	20	C121	1 0 0 0 1	unit assumed, *sic*
6.404E-01	4.807E+01	25	M346	2 1 1 1 2	

91. $C_2H_5NO_2$
Methyl carbamate
Carbamidsaeure-methyl ester
Methyl urethane
RN: 598-55-0 **MP** (°C)**:** 52
MW: 75.07 **BP** (°C)**:** 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.125E+00	6.850E+02	11	F300	1 0 0 0 2	
9.119E+00	6.845E+02	11	I314	0 0 0 0 0	
9.200E+00	6.906E+02	15.50	F001	1 0 1 0 2	
5.462E+00	4.100E+02	15.50	F300	1 0 0 0 1	

92. $C_2H_5NO_2$
Glycolamide
2-Hydroxyacetamide
2-Hydroxyacetimidic acid
Glycolic amide
Glycolic acid amide
RN: 598-42-5 **MP** (°C)**:**
MW: 75.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.509E+00	4.135E+02	25	M008	1 0 0 0 2	

93. C_2H_5NS
Thiacetamide
Thioessigsaeureamid
Thioacetamide
Acetothioamide
Ethanethioamide
RN: 62-55-5 **MP** (°C)**:** 113
MW: 75.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.865E+00	1.402E+02	25	I310	0 0 0 0 0	

94. $C_2H_5N.2H_2O$
Ethyleneimine (dihydrate)
Aziridine (dihydrate)
RN: 151-56-4 **MP** (°C)**:**
MW: 79.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-02	5.411E+00	20	P315	0 0 0 0 0	

95. $C_2H_5N_3O_2$
Methylnitrosourea
MNU
Nitrosomethylurea
RN: 684-93-5 **MP** (°C)**:** 123
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.443E+01	24	M031	1 1 1 1 1	
1.413E-01	1.456E+01	ns	R424	0 0 0 0 0	

96. $C_2H_5N_3O_2$
Biuret
Carbamylurea
RN: 108-19-0 **MP** (°C)**:**
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-01	1.200E+01	0	F300	1 0 0 0 2	
1.475E-01	1.520E+01	15	F300	1 0 0 0 2	
3.104E+00	3.200E+02	106	F300	1 0 0 0 1	

97. $C_2H_5N_5O_3$
N-Methyl-*N′*-nitro-*N*-nitrosoguanidine
MNNG
1-Methyl-3-nitro-1-nitrosoguanidine
RN: 70-25-7 **MP** (°C)**:** 118
MW: 147.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.38E-02	<4.98E+00	ns	I307	0 0 0 0 0	

98. $C_2H_5O_5P$
Phosphoacetic acid
Phosphor carboxymethyl-phosphonsaeure
Phosphonoacetic acid
RN: 4408-78-0 **MP** (°C)**:** 144.5
MW: 140.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E+00	3.920E+02	0	F300	1 0 0 0 2	
2.800E+00	3.921E+02	0	N028	1 0 0 0 2	

99. $C_2H_5O_5As$
Arsonoacetic acid
Arsono-essigsaeure
RN: 107-38-0 **MP** (°C)**:** 152
MW: 183.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E+00	4.000E+02	18	F300	1 0 0 0 1	

100. C_2H_6
Ethane
Aethan
RN: 74-84-0 **MP** (°C)**:** –172
MW: 30.07 **BP** (°C)**:** –88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-01	7.779E+00	0	C075	1 0 1 0 1	
4.157E-03	1.250E-01	0	F300	1 0 0 0 2	
3.601E-03	1.083E-01	4.99	C115	2 0 2 2 2	
2.903E-03	8.730E-02	9.99	C115	2 0 2 2 2	
2.465E-03	7.413E-02	14.99	C115	2 0 2 2 2	

(*continued*)

100. C_2H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-03	6.682E-02	19.8	G058	1 0 0 0 2	
2.129E-03	6.401E-02	19.99	C115	2 0 2 2 2	
1.929E-03	5.800E-02	20	F300	1 0 0 0 1	
1.850E-03	5.563E-02	24.99	C115	2 0 2 2 2	
2.009E-03	6.040E-02	25	M001	2 1 2 2 2	
2.009E-03	6.040E-02	25	M002	2 2 1 2 2	
1.760E-03	5.292E-02	25	M102	1 2 2 1 2	
1.620E-03	4.871E-02	29.99	C115	2 0 2 2 2	
7.981E-04	2.400E-02	60	F300	1 0 0 0 1	

101. C_2H_6O

Methyl ether
Dimethyl ether
Dimethylaether

RN: 115-10-6 **MP** (°C)**:** –138
MW: 46.07 **BP** (°C)**:** –23.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.476E+00	6.800E+01	18	F300	1 0 0 0 1	
5.669E+00	2.612E+02	24	M065	1 0 2 1 2	

102. $C_2H_6O_2$

Ethylene glycol
Glycol
1,2-Ethandiol

RN: 107-21-1 **MP** (°C)**:** –13
MW: 62.07 **BP** (°C)**:** 197.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.710E+00	4.165E+02	4.50	C022	1 2 0 0 2	
5.562E-01	3.452E+01	25	B004	0 0 0 0 0	

103. $C_2H_6O_3S$

Methyl methanesulphonate
Methyl mesylate
Methanesulfonic acid methyl ester

RN: 66-27-3 **MP** (°C)**:** 20
MW: 110.13 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.513E+00	1.667E+02	25	I310	0 0 0 0 0	

104. $C_2H_6O_4S$

Dimethyl sulfate
Sulfuric acid dimethyl ester

RN: 77-78-1 **MP** (°C)**:** –27
MW: 126.13 **BP** (°C)**:** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-01	2.800E+01	18	B078	1 0 0 0 1	
2.159E-01	2.724E+01	18	D049	1 2 0 0 1	

105. C_2H_7N

Ethylamine
Aethylamin

RN: 75-04-7 **MP** (°C)**:** –81
MW: 45.08 **BP** (°C)**:** 16.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.686E-02	1.211E+00	25	B004	0 0 0 0 0	

106. $C_2H_7NO_3S$

Taurine
Taurin

RN: 107-35-7 **MP** (°C)**:** 328
MW: 125.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-01	3.754E+01	0	M043	1 0 0 0 1	
4.523E-01	5.660E+01	10	M043	1 0 0 0 1	
4.842E-01	6.060E+01	12	F300	1 0 0 0 2	
3.919E-01	4.905E+01	15	G081	1 0 1 1 2	
6.448E-01	8.070E+01	20	F300	1 0 0 0 2	
6.463E-01	8.088E+01	20	M043	1 0 0 0 1	
4.700E-01	5.882E+01	24	D031	1 0 0 0 2	
7.580E-01	9.486E+01	25	D041	1 0 0 0 2	
8.815E-01	1.103E+02	30	M043	1 0 0 0 2	
1.149E+00	1.438E+02	40	M043	1 0 0 0 2	
1.719E+00	2.151E+02	60	M043	1 0 0 0 2	
1.985E+00	2.484E+02	70	F300	1 0 0 0 2	
2.105E+00	2.634E+02	75	D041	1 0 0 0 2	
2.217E+00	2.775E+02	80	M043	1 0 0 0 2	
2.506E+00	3.137E+02	100	M043	1 0 0 0 2	

107. $C_2H_7O_2As$
Cacodylic acid
Dimethylarsinsaeure
Kakodylsaeure
Arsine oxide, hydroxydimethyl-
Cacodylic acid
RN: 75-60-5 **MP** (°C)**:** 195
MW: 138.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.899E+00	4.001E+02	20	B200	1 0 0 0 2	
3.287E+00	4.536E+02	22	B185	0 0 0 0 0	
3.290E+00	4.540E+02	22	F300	1 0 0 0 2	
4.961E+00	6.845E+02	25	D305	1 0 0 0 2	
1.449E+01	2.000E+03	25	M161	1 0 0 0 0	

108. C_2H_7As
Ethylarsine
Aethylarsin
Arsen
RN: 593-59-9 **MP** (°C)**:**
MW: 106.00 **BP** (°C)**:** 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	1.300E-01	19	F300	1 0 0 0 1	

109. $C_2Cl_2F_4$
1,2-Dichlorotetrafluoroethane
CFC-114
sym-Dichlorotetrafluoroethane
Halon 242
1,2-Dichloro-1,1,2,2-tetrafluoroethane
Cryofluorane
RN: 76-14-2 **MP** (°C)**:** –94
MW: 170.92 **BP** (°C)**:** 3.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-04	1.300E-01	25	R048	0 0 0 0 0	

110. $C_2Cl_3F_3$
1,1,2-Trichloro-1,2,2-trifluoroethane
Freon 113
Fluorocarbon 113
Halocarbon 113
RN: 76-13-1 **MP** (°C)**:** –36.4
MW: 187.38 **BP** (°C)**:** 47.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.071E-04	1.700E-01	25	R048	0 0 0 0 0	

111. C_2Cl_4
Tetrachloroethylene
Ethylene tetrachloride
Perchloroethylene
Tetrachloroethene
Tetrachloro-ethylene
PERC
RN: 127-18-4 **MP** (°C)**:** –22
MW: 165.83 **BP** (°C)**:** 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-03	2.000E-01	20	C094	1 0 1 0 2	
1.206E-03	2.000E-01	20	C121	0 0 0 0 0	unit assumed, *sic*
9.045E-04	1.500E-01	20	M133	1 0 0 0 2	
9.045E-04	1.500E-01	20	P046	1 0 0 0 0	
9.044E-04	1.500E-01	25	A094	1 0 0 0 1	
2.920E-03	4.842E-01	25	B173	2 0 2 2 2	
1.206E-03	2.000E-01	25	C119	2 2 2 2 2	
2.412E-03	4.000E-01	25	F071	1 1 2 1 2	
9.044E-04	1.500E-01	25	G056	1 0 0 0 2	
9.045E-04	1.500E-01	25	M037	1 1 0 0 1	
9.045E-04	1.500E-01	25	M368	1 0 0 0 1	
9.044E-04	1.500E-01	25	N034	1 0 0 0 1	
2.412E-03	4.000E-01	ns	M344	0 0 0 0 2	
9.044E-04	1.500E-01	ns	O006	0 0 0 0 1	

112. C_2Cl_6
Hexachloroethane
1,1,1,2,2,2-Hexachloroethane
Avlothane
Distopin
Distopan
Distokal
RN: 67-72-1 **MP** (°C)**:** 187
MW: 236.74 **BP** (°C)**:** 186.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-05	7.700E-03	20	M339	2 2 2 2 1	
2.112E-04	5.000E-02	22.3	M037	1 1 0 0 0	
1.148E-04	2.718E-02	ns	R427	0 0 0 0 0	

113. C_2N_2
Cyanogen
Dicyan
RN: 460-19-5 **MP** (°C)**:**
MW: 52.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E+01	8.182E+02	20	F300	1 0 0 0 1	

114. $C_2N_4S_2$
Cyanogen azidodithiocarbonate
RN: **MP** (°C)**:**
MW: 144.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-02	1.500E+00	0	A055	0 0 0 0 2	

115. $C_2N_6S_4$
Thioperoxydicarbonic diazide
Azidoschwefel-kohlenstoff
Azidocarbonicdisulfide
RN: 148832-09-1 **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E-03	3.000E-01	25	F300	1 0 0 0 0	

116. $C_3H_2Cl_2N_2O_2$
1,3-Dichlorohydantoin
2,4-Imidazolidinedione, 1,3-dichloro-
RN: 2958-99-8 **MP** (°C)**:**
MW: 168.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.114E-02	6.951E+00	20	B080	1 0 1 1 0	
8.171E-02	1.381E+01	40	B080	1 0 1 1 1	

117. $C_3H_2N_2$
Malononitrile
Malonsaeure-dinitril
RN: 109-77-3 **MP** (°C)**:** 32
MW: 66.06 **BP** (°C)**:** 218.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E+00	1.176E+02	20	F300	1 0 0 0 2	
1.778E+00	1.175E+02	ns	R424	0 0 0 0 0	

118. $C_3H_2N_2O_3$
Parabanic acid
Parabansaeure
RN: 120-89-8 **MP** (°C)**:**
MW: 114.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.945E-01	4.500E+01	8	F300	1 0 0 0 1	

119. $C_3H_3Cl_3O_3$
β,β,β-Trichlorolactic acid
β,β,β-Trichlor-milchsaeure
RN: 599-01-9 **MP** (°C)**:**
MW: 193.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E+00	4.380E+02	25	F300	1 0 0 0 2	

120. C_3H_3N

Acrylonitrile
Propenitrile

RN: 107-13-1 **MP** (°C)**:** –83.5
MW: 53.06 **BP** (°C)**:** 77.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E+00	6.716E+01	0	D046	0 0 0 0 0	
1.266E+00	6.716E+01	0	D046	2 2 0 0 1	EFG
1.282E+00	6.803E+01	20	D046	0 0 0 0 0	
1.282E+00	6.803E+01	20	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	0 0 0 0 0	
1.298E+00	6.890E+01	25	L096	1 2 0 2 1	
1.413E+00	7.500E+01	25	M161	1 0 0 0 1	
1.315E+00	6.977E+01	28	D046	2 2 0 0 1	EFG
1.347E+00	7.149E+01	36	D046	2 2 0 0 1	EFG
1.364E+00	7.236E+01	39	D046	2 2 0 0 1	EFG
1.388E+00	7.365E+01	41	D046	2 2 0 0 2	EFG
1.508E+00	8.004E+01	49	D046	2 2 0 0 1	EFG
1.508E+00	8.004E+01	53	D046	2 2 0 0 1	EFG
1.540E+00	8.173E+01	59	D046	2 2 0 0 1	EFG
1.603E+00	8.509E+01	63	D046	2 2 0 0 1	EFG
1.760E+00	9.338E+01	65	A324	2 2 2 1 2	
1.651E+00	8.759E+01	68	D046	2 2 0 0 0	EFG
1.721E+00	9.132E+01	72	D046	2 2 0 0 0	EFG
1.869E+00	9.918E+01	80	D046	2 2 0 0 0	EFG
1.974E+00	1.047E+02	85	D046	2 2 1 1 0	EFG
2.124E+00	1.127E+02	90	D046	2 2 1 1 0	EFG

121. $C_3H_3NOS_2$

Rhodanine
Rhodanin

RN: 141-84-4 **MP** (°C)**:** 170
MW: 133.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E-02	2.250E+00	25	F300	1 0 0 0 2	

122. $C_3H_3N_3O_3$
Cyanuric acid
Cyanursaeure
Isocyanuric acid
Isocyanursaeure
RN: 108-80-5 **MP** (°C)**:**
MW: 129.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	2.969E+00	2	B193	1 2 0 0 1	
3.874E-02	5.000E+00	20	F300	1 0 0 0 0	
2.009E-02	2.593E+00	25	B384	0 0 0 0 0	

123. $C_3H_3N_3O_3$
Cyamelide
Cyamelid
RN: 462-02-2 **MP** (°C)**:**
MW: 129.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.747E-04	1.000E-01	15	F300	1 0 0 0 0	

124. $C_3H_3N_3S_3$
Trithiocyanuric acid
s-Triazine-2,4,6-trithiol
Trimercapto-*s*-triazine
RN: 638-16-4 **MP** (°C)**:**
MW: 177.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.399E-01	25	B384	0 0 0 0 0	

125. C_3H_4
Propyne
Methyl acetylene
Methylacetylene
RN: 74-99-7 **MP** (°C)**:** –101
MW: 40.07 **BP** (°C)**:** –23.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.085E-02	3.239E+00	21	I011	1 2 2 1 2	
9.085E-02	3.640E+00	25	M001	2 1 2 2 2	
5.488E-02	2.199E+00	38	I011	1 2 2 1 1	
3.606E-02	1.445E+00	54	I011	1 2 2 1 1	
2.220E-02	8.895E-01	71	I011	1 2 2 1 1	
8.886E-03	3.560E-01	88	I011	1 2 2 1 1	

126. $C_3H_4ClN_5$
Desethyl simazine
Amino-2-chloro-6-ethylamino-*s*-triazine
6-Chloro-*N*-ethyl-1,3,5-triazine-2,4-diamine
RN: 1007-28-9 **MP** (°C)**:**
MW: 145.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.747E-01	2	B193	1 1 0 0 0	

127. $C_3H_4Cl_2$
1,2-Dichloropropene
Dichloropropylene
RN: 26952-23-8 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

128. $C_3H_4Cl_2$
trans-1,3-Dichloropropene
1,3-Dichloropropylene (*trans*)
trans-1,3-Dichloropropylene
1,3-Dichloropropene
RN: 542-75-6 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.703E-03	2.999E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
9.011E-03	1.000E+00	20	M161	1 0 0 0 0	
1.071E-02	1.188E+00	30	M300	1 1 2 2 2	

129. $C_3H_4Cl_2$
cis-1,3-Dichloropropene
1,3-Dichloropropropylene (*cis*)
cis-1,3-Dichloropropylene
cis 1,3-Dichloro-propene
cis-1,3-Dichloro-1-propene
(Z)-1,3-Dichloropropene
RN: 10061-01-5 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	2.700E+00	20	G080	1 0 0 0 1	
9.651E-03	1.071E+00	30	M300	1 1 2 2 2	
8.211E-03	9.112E-01	30	M311	1 1 2 2 2	

130. $C_3H_4Cl_2$

trans-1,3-Dichloro-propene
trans-1,3-Dichloro-1-propene
(E)-1,3-Dichloro-1-propene
E-1,3-Dichloropropene

RN: 10061-02-6 **MP** (°C)**:**
MW: 110.97 **BP** (°C)**:** 111

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	2.800E+00	20	G080	1 0 0 0 1	

131. $C_3H_4Cl_2O_2$

Dalapon
α,α-Dichlor-propionsaeure

RN: 75-99-0 **MP** (°C)**:**
MW: 142.97 **BP** (°C)**:** 187.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E+00	5.020E+02	25	M161	1 0 0 0 2	
3.511E+00	5.020E+02	ns	K138	0 0 0 0 1	

132. $C_3H_4N_2O$

Cyanoacetamide
Cyanessigsaeure-amid

RN: 107-91-5 **MP** (°C)**:**
MW: 84.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E+00	1.300E+02	20	F300	1 0 0 0 1	

133. $C_3H_4N_2O_2$

Hydantoin
2,4-Imidazolidinedione

RN: 461-72-3 **MP** (°C)**:** 220
MW: 100.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E+00	2.946E+02	100	F300	1 0 0 0 2	
3.970E-01	3.973E+01	ns	M025	0 2 0 1 2	

134. $C_3H_4N_2O_3S$

2-Imidazole sulfonic acid
Imidazol-sulfosaeure-(2)
RN: 53744-47-1 **MP** (°C)**:**
MW: 148.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.009E-01	7.420E+01	20	F300	1 0 0 0 2	

135. $C_3H_4N_4O_2$

Ammelide
2,4-Dihydroxy-6-amino-1,3,5-triazine
RN: 645-93-2 **MP** (°C)**:**
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.685E-02	2	B193	1 2 0 0 0	

136. C_3H_4O

Acrolein
2-Propenal
Acrylaldehyde
RN: 107-02-8 **MP** (°C)**:** –88.0
MW: 56.06 **BP** (°C)**:** 52.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.690E+00	4.872E+02	0	B111	1 0 0 1 1	Quinol as a stabilizer
3.764E+00	2.110E+02	20	F300	1 0 0 0 2	
3.071E+00	1.722E+02	20	M161	1 0 0 0 1	
8.522E+00	4.778E+02	32.50	B111	1 0 0 1 2	Quinol as a stabilizer
8.429E+00	4.726E+02	44.40	B111	1 0 0 1 2	Quinol as a stabilizer
8.339E+00	4.675E+02	50	B111	1 0 0 1 2	Quinol as a stabilizer
8.288E+00	4.647E+02	53	B111	1 0 0 1 2	Quinol as a stabilizer
7.889E+00	4.423E+02	74.50	B111	1 0 0 1 2	Quinol as a stabilizer
7.338E+00	4.114E+02	82	B111	1 0 0 1 2	Quinol as a stabilizer
7.013E+00	3.932E+02	84	B111	1 0 0 1 2	Quinol as a stabilizer
6.597E+00	3.699E+02	87.80	B111	1 0 0 1 2	Quinol as a stabilizer
6.417E+00	3.598E+02	88	B111	1 0 0 1 2	Quinol as a stabilizer
5.096E+00	2.857E+02	ns	B185	0 0 0 0 0	
3.567E+00	2.000E+02	ns	B200	0 0 0 0 0	

137. $C_3H_4O_4$
Malonic acid
Acide malonique
Malonsaeure
RN: 141-82-2 **MP** (°C)**:** 135
MW: 104.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.645E+00	3.793E+02	0	F300	1 0 0 0 2	
5.871E+00	6.110E+02	0	L041	1 0 0 1 2	
4.990E+00	5.192E+02	0	M043	1 0 0 0 2	
5.871E+00	6.110E+02	0	M051	1 0 0 0 2	
4.743E+00	4.936E+02	4.99	A339	0 0 0 0 0	
5.427E+00	5.648E+02	10	K077	1 2 2 2 2	average of 3
5.395E+00	5.614E+02	10	M043	1 0 0 0 2	
4.888E+00	5.087E+02	9.99	A339	0 0 0 0 0	
5.034E+00	5.238E+02	14.99	A339	0 0 0 0 0	
5.608E+00	5.836E+02	15	K077	1 2 2 2 2	
6.746E+00	7.020E+02	15	L041	1 0 0 1 2	
6.746E+00	7.020E+02	15	M051	1 0 0 0 2	
5.728E+00	5.961E+02	18	K077	1 2 2 2 2	
5.198E+00	5.409E+02	19.99	A339	0 0 0 0 0	
7.063E+00	7.350E+02	20	L041	1 0 0 1 2	
5.811E+00	6.047E+02	20	M043	1 0 0 0 2	
4.067E+00	4.232E+02	20	M171	1 0 0 0 2	
2.670E+00	2.778E+02	20	S006	1 0 0 0 2	
5.928E+00	6.169E+02	24	K077	1 2 2 2 2	
5.354E+00	5.571E+02	24.99	A339	0 0 0 0 0	
4.221E+00	4.393E+02	25	F300	1 0 0 0 2	
5.990E+00	6.233E+02	25	K077	1 2 2 2 2	
7.332E+00	7.630E+02	25	M051	1 0 0 0 2	
5.494E+00	5.717E+02	29.99	A339	0 0 0 0 0	
6.178E+00	6.429E+02	30	M043	1 0 0 0 2	
5.638E+00	5.867E+02	34.99	A339	0 0 0 0 0	
7.938E+00	8.260E+02	35	L041	1 0 0 1 2	
5.800E+00	6.035E+02	39.99	A339	0 0 0 0 0	
6.530E+00	6.795E+02	40	M043	1 0 0 0 2	
5.913E+00	6.153E+02	44.99	A339	0 0 0 0 0	
6.028E+00	6.273E+02	49.99	A339	0 0 0 0 0	
8.898E+00	9.260E+02	50	L041	1 0 0 1 2	
8.898E+00	9.260E+02	50	M051	1 0 0 0 2	
6.895E+00	7.175E+02	53	K077	1 2 2 2 2	
6.182E+00	6.433E+02	54.99	A339	0 0 0 0 0	
6.328E+00	6.585E+02	59.99	A339	0 0 0 0 0	
7.158E+00	7.449E+02	60	M043	1 0 0 0 2	
6.451E+00	6.713E+02	64.99	A339	0 0 0 0 0	
9.831E+00	1.023E+03	65	L041	1 0 0 1 2	
7.878E+00	8.198E+02	80	M043	1 0 0 0 2	
8.267E+00	8.603E+02	93	K077	1 2 2 2 2	
8.554E+00	8.901E+02	100	M043	1 0 0 0 2	
9.610E+00	1.000E+03	132	K077	1 2 2 2 2	
1.441E+01	1.500E+03	ns	D072	0 0 0 0 1	

138. C_3H_5Br
Allyl bromide
3-Bromopropene
RN: 106-95-6 **MP** (°C)**:** –119
MW: 120.98 **BP** (°C)**:** 71.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.170E-02	3.835E+00	25	M342	1 0 1 1 2	

139. $C_3H_5Bvr_2Cl$
1,2-Dibromo-3-chloropropane
1-Chloro-2,3-dibromopropane
Nemagon
RN: 96-12-8 **MP** (°C)**:**
MW: 236.34 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.204E-03	1.230E+00	20	G080	1 0 0 0 1	
4.227E-03	9.990E-01	20	P081	1 0 0 0 0	
4.227E-03	9.990E-01	ns	I316	0 0 0 0 0	
4.227E-03	9.990E-01	ns	M061	0 0 0 0 0	
4.231E-03	1.000E+00	rt	M161	0 0 0 0 0	

140. C_3H_5Cl
Allyl chloride
3-Chloro-1-propene
RN: 107-05-1 **MP** (°C)**:** –134
MW: 76.53 **BP** (°C)**:** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-02	3.587E+00	20	G056	1 0 0 0 2	
1.305E-02	9.990E-01	ns	N034	0 0 0 0 0	

141. C_3H_5ClO
Chloroacetone
1-Chloro-2-propanone
Chloraceton
RN: 78-95-5 **MP** (°C)**:** –44.5
MW: 92.53 **BP** (°C)**:** 119.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.924E-01	8.257E+01	ns	N034	0 0 0 0 0	

142. C_3H_5ClO

Epichlorohydrin
Epichloridrina

RN: 106-89-8 **MP** (°C)**:** –25.6
MW: 92.53 **BP** (°C)**:** 117.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-01	6.086E+01	0	L061	1 2 2 1 2	
6.615E-01	6.121E+01	10	L061	1 2 2 1 2	
6.501E-01	6.015E+01	20	I313	0 0 0 0 0	
6.692E-01	6.191E+01	30.20	L061	1 2 2 1 2	
7.568E-01	7.003E+01	52	L061	1 2 2 1 2	
8.421E-01	7.792E+01	65	L061	1 2 2 1 2	
9.232E-01	8.542E+01	72	L061	1 2 2 1 2	
1.024E+00	9.478E+01	80.20	L061	1 2 2 1 2	

143. $C_3H_5Cl_2NO_2$

1,1-Dichloro-1-nitropropane
Propane, 1,1-dichloro-1-nitro-

RN: 595-44-8 **MP** (°C)**:**
MW: 157.98 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.149E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, *sic*

144. $C_3H_5Cl_3$

1,2,3-Trichloropropane
Allyl trichloride
Trichlorohydrin
Glycerol trichlorohydrin

RN: 96-18-4 **MP** (°C)**:** –14
MW: 147.43 **BP** (°C)**:** 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-02	1.900E+00	ns	H123	0 0 0 0 0	

145. $C_3H_5IO_2$

β-Iodopropionic acid
β-Iod-propionsaeure

RN: 141-76-4 **MP** (°C)**:** 81.5
MW: 199.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.715E-01	7.430E+01	25	F300	1 0 0 0 2	

146. C_3H_5N
Propionitrile
Propionsaeure-nitril
n-Propionitrile
RN: 107-12-0 **MP** (°C)**:** –93
MW: 55.08 **BP** (°C)**:** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.151E-02	3.388E+00	25	B004	0 0 0 0 0	

147. C_3H_5N
Ethyl isocyanide
Ethane, isocyano-
RN: 624-79-3 **MP** (°C)**:**
MW: 55.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.814E-02	9.990E-01	ns	L055	0 0 0 0 1	

148. C_3H_5NO
Acrylamide
2-Propenamide
RN: 79-06-1 **MP** (°C)**:** 84
MW: 71.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.299E+00	3.056E+02	0	M147	0 2 1 1 0	EFG
4.690E+00	3.333E+02	10	M147	0 2 1 1 0	EFG
5.220E+00	3.711E+02	20	M147	0 2 1 1 0	EFG
5.695E+00	4.048E+02	30	M147	0 2 1 1 0	EFG
6.075E+00	4.318E+02	40	M147	0 2 1 1 0	EFG
6.253E+00	4.444E+02	50	M147	0 2 1 1 0	EFG
6.625E+00	4.709E+02	60	M147	0 2 1 1 0	EFG
7.034E+00	5.000E+02	80	M147	0 2 1 1 0	EFG

149. $C_3H_5NO_3$
Formylglycine
N-Formyl glycine
RN: 2491-15-8 **MP** (°C)**:**
MW: 103.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E+00	1.906E+02	25	M024	1 2 0 1 2	
1.849E+00	1.906E+02	ns	M025	0 2 0 1 2	

150. $C_3H_5N_3O$
Ethylnitrosocyanamide
ENC
RN: 38434-77-4 **MP** (°C)**:**
MW: 99.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.387E+01	24	M031	1 1 1 1 1	

151. $C_3H_5N_3O_9$
Nitroglycerin
Nitroglycerol
RN: 55-63-0 **MP** (°C)**:** 13.5
MW: 227.09 **BP** (°C)**:** 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.629E-03	1.278E+00	15	L063	2 0 1 1 2	
7.926E-03	1.800E+00	20	F300	1 0 0 0 1	
6.069E-03	1.378E+00	20	L063	2 0 1 1 2	
5.504E-03	1.250E+00	25	P312	0 0 0 0 0	
6.595E-03	1.498E+00	30	L063	2 0 1 1 2	
7.342E-03	1.667E+00	40	L063	2 0 1 1 2	
8.570E-03	1.946E+00	50	L063	2 0 1 1 2	
1.041E-02	2.364E+00	60	L063	2 0 1 1 2	
1.265E-02	2.872E+00	70	L063	2 0 1 1 2	
1.518E-02	3.448E+00	80	L063	2 0 1 1 2	

152. $C_3H_5N_5O$
Ammeline
Ammelin
RN: 645-92-1 **MP** (°C)**:**
MW: 127.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.626E-02	2	B193	1 1 0 0 0	
5.901E-04	7.500E-02	23	F300	1 0 0 0 1	
2.486E-03	3.160E-01	100	F300	1 0 0 0 2	

153. C_3H_6

Cyclopropane
Trimethylene

RN: 75-19-4 **MP** (°C)**:** –127
MW: 42.08 **BP** (°C)**:** –33

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.461E-02	1.036E+00	5.05	Z008	2 1 2 2 2	at 97.26 kPa
1.281E-02	5.390E-01	20	R060	0 0 0 0 0	
1.754E-02	7.382E-01	21	I017	1 2 2 1 2	at 16.9 psia
1.103E-02	4.640E-01	25	R060	0 0 0 0 0	
9.315E-03	3.920E-01	30	R060	0 0 0 0 0	
8.983E-03	3.780E-01	31	R060	0 0 0 0 0	
7.723E-03	3.250E-01	35	R060	0 0 0 0 0	
1.083E-02	4.557E-01	38	I017	1 2 2 1 2	at 17.0 psia
6.844E-03	2.880E-01	39	R060	0 0 0 0 0	
5.917E-03	2.490E-01	45	R060	0 0 0 0 0	
8.386E-03	3.529E-01	71	I017	1 2 2 1 2	at 19.9 psia
3.999E-03	1.683E-01	104	I017	1 2 2 1 2	at 24.9 psia
5.896E+00	2.481E+02	ns	R028	0 0 0 0 0	

154. C_3H_6

Propylene
Methyl ethylene
Propene

RN: 115-07-1 **MP** (°C)**:** –185
MW: 42.08 **BP** (°C)**:** –48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.139E-02	9.000E-01	0	F300	1 0 0 0 1	
7.553E-03	3.178E-01	21	A052	1 1 1 2 2	smoothed
7.842E-03	3.300E-01	25	F300	1 0 0 0 1	
4.753E-03	2.000E-01	25	M001	2 1 2 2 2	
4.221E-03	1.776E-01	38	A052	1 1 1 2 1	smoothed
2.333E-03	9.818E-02	54	A052	1 1 1 2 1	smoothed
1.500E-03	6.312E-02	71	A052	1 1 1 2 1	smoothed
7.222E-04	3.039E-02	88	A052	1 1 1 2 1	smoothed

155. C_3H_6BrCl

1-Bromo-3-chloropropane
w-Chlorobromopropane
3-Bromopropyl chloride
3-Chloro-1-bromopropane

RN: 109-70-6 **MP** (°C)**:** –58.9
MW: 157.44 **BP** (°C)**:** 143.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-02	2.236E+00	25	M342	1 0 1 1 2	

156. $C_3H_6BrNO_4$
Bronopol
2-Bromo-2-nitropropane-1,3-diol
RN: 52-51-7 **MP** (°C)**:** 130
MW: 199.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+00	2.000E+02	22	M161	1 0 0 0 1	

157. $C_3H_6Br_2$
Trimethylene bromide
1,3-Dibromopropane
RN: 109-64-8 **MP** (°C)**:** –36
MW: 201.90 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.406E-03	1.697E+00	20	C121	1 0 0 0 1	unit assumed, *sic*

158. $C_3H_6ClNO_2$
1-Chloro-1-nitropropane
Propane, 1-chloro-1-nitro-
RN: 600-25-9 **MP** (°C)**:**
MW: 123.54 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	C121	1 0 0 0 0	unit assumed, *sic*
4.027E-02	4.975E+00	20	M061	1 0 0 0 0	

159. $C_3H_6ClNO_2$
1-Chloro-2-nitropropane
Propane, 1-chloro-2-nitro-
RN: 37809-02-2 **MP** (°C)**:**
MW: 123.54 **BP** (°C)**:** 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	M061	1 0 0 0 0	

160. $C_3H_6Cl_2$
Propylene dichloride
1,2-Dichlor-propan
1,2-Dichloropropane
Propylene chloride
Dichloropropane
RN: 78-87-5 **MP** (°C)**:** –100.3
MW: 112.99 **BP** (°C)**:** 96.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.160E-02	3.570E+00	20	C094	1 0 1 0 2	
2.383E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
2.390E-02	2.700E+00	20	F300	1 0 0 0 1	
2.390E-02	2.700E+00	20	M037	1 1 0 0 1	
2.383E-02	2.693E+00	20	M061	1 0 0 0 1	
2.295E-02	2.593E+00	20	M062	1 0 0 0 1	
2.390E-02	2.700E+00	20	M161	1 0 0 0 1	
2.500E-02	2.825E+00	20	M312	1 0 0 0 1	
2.383E-02	2.693E+00	20	N034	1 0 0 0 1	
2.478E-02	2.800E+00	25	F300	1 0 0 0 1	
2.480E-02	2.802E+00	25	G038	1 2 2 2 2	
2.480E-02	2.802E+00	25	G053	2 1 2 1 2	
2.295E-02	2.593E+00	25	G056	1 0 0 0 2	
2.142E-02	2.420E+00	30	M300	1 1 2 2 2	
1.831E-02	2.069E+00	30	M311	1 1 2 2 2	

161. $C_3H_6Cl_2$
1,3-Dichloropropane
1,3-Dichlor-propan
RN: 142-28-9 **MP** (°C)**:** –99
MW: 112.99 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-02	2.892E+00	20	C121	1 0 0 0 1	unit assumed, *sic*
2.416E-02	2.730E+00	25	F300	1 0 0 0 2	
2.430E-02	2.746E+00	25	G038	1 2 2 2 2	
2.430E-02	2.746E+00	25	G053	2 1 2 1 2	
9.027E-03	1.020E+00	30	M311	1 1 2 2 2	

162. $C_3H_6Cl_2O$
1,3-Dichloro-2-propanol
1,3-Dichlor-propanol-(2)
RN: 96-23-1 **MP** (°C)**:** –4
MW: 128.99 **BP** (°C)**:** 174.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.675E-01	9.900E+01	19	F300	1 0 0 0 1	
6.984E-01	9.008E+01	19	N034	1 0 0 0 1	
1.124E+00	1.450E+02	72	F300	1 0 0 0 2	

163. $C_3H_6N_2O_2$
Malonic acid diamide
Malonsaeure-diamid
Malonamide
Malonodiamide
Propanediamide
RN: 108-13-4 **MP** (°C)**:** 170
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.513E-01	7.670E+01	8	F300	1 0 0 0 2	
7.830E-03	7.994E-01	ns	L055	0 0 0 0 1	

164. $C_3H_6N_2O_2$
Methylglyoxime
Methylglyoxim
RN: 1804-15-5 **MP** (°C)**:**
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-01	4.600E+01	26	F300	1 0 0 0 1	
7.444E-01	7.600E+01	40	F300	1 0 0 0 1	

165. $C_3H_6N_2O_2$
Methylnitrosoacetamide
MNA
RN: 7417-67-6 **MP** (°C)**:**
MW: 102.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-01	1.736E+01	24	M031	1 1 1 1 1	

166. $C_3H_6N_2O_2$
1-Acetylurea
Acetylharnstoff
RN: 591-07-1 **MP** (°C)**:** 218
MW: 102.09 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-01	1.300E+01	15	F300	1 0 0 0 1	

167. $C_3H_6N_2O_3$
Hydantoic acid
N-(Carboxymethyl)urea
N-Carbamoylglycine
Carbamoylglycine
Glycoluric acid
RN: 462-60-2 **MP** (°C)**:**
MW: 118.09 **BP** (°C)**:**

Solub ility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E-01	3.010E+01	20	F300	1 0 0 0 2	
3.290E-01	3.885E+01	25	M024	1 2 0 1 2	
3.290E-01	3.885E+01	ns	M025	0 2 0 1 2	

168. $C_3H_6N_2O_7$
Glycerol 1,2-dinitrate
1,2,3-Propanetriol 1,2-dinitrate
1,2-Dinitroglycerol
RN: 131287-51-9 **MP** (°C)**:**
MW: 182.09 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.386E-01	6.165E+01	20	D013	1 0 1 1 2	

169. $C_3H_6N_2O_7$
Glycerol 1,3-dinitrate
Glycerol-α,α′-dinitrate
Glycerin-α,α′-dinitrate
RN: 623-87-0 **MP** (°C)**:** 26
MW: 182.09 **BP** (°C)**:** 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.993E-01	7.270E+01	20	D013	1 0 1 1 2	

170. $C_3H_6N_2S$
Ethylenethiourea
Mercaptoimidazoline
Mercozen
RN: 96-45-7 **MP** (°C)**:** 203
MW: 102.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-01	1.961E+01	30	I310	0 0 0 0 0	
8.082E-01	8.257E+01	60	I310	0 0 0 0 0	
2.991E+00	3.056E+02	90	I310	0 0 0 0 0	

171. $C_3H_6N_4Hg$

Methylmercuridicyanodiamide
Panogen

RN: 502-39-6 **MP** (°C)**:** 156
MW: 298.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.265E-02	2.170E+01	20	M061	1 0 0 0 2	
7.265E-02	2.170E+01	rt	M161	0 0 0 0 2	

172. $C_3H_6N_6$

Melamine
1,3,5-Triazine-2,4,6-triamine
Cymel

RN: 108-78-1 **MP** (°C)**:**
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.503E-03	1.199E+00	0	M043	1 0 0 0 1	
1.000E-02	1.261E+00	2	B193	1 1 0 0 1	
1.425E-02	1.797E+00	10	M043	1 0 0 0 1	
2.561E-02	3.230E+00	19.90	C023	2 2 0 1 2	
2.135E-02	2.693E+00	20	M043	1 0 0 0 1	
3.316E-02	4.182E+00	30	M043	1 0 0 0 1	
4.651E-02	5.865E+00	34.90	C023	2 2 0 1 2	
5.590E-02	7.050E+00	40	M043	1 0 0 0 1	
8.200E-02	1.034E+01	49.80	C023	2 2 0 1 2	
1.172E-01	1.478E+01	60	M043	1 0 0 0 1	
1.325E-01	1.672E+01	64.10	C023	2 2 0 1 2	
1.836E-01	2.315E+01	74.50	C023	2 2 0 1 2	
2.160E-01	2.724E+01	80	M043	1 0 0 0 1	
2.421E-01	3.054E+01	83.50	C023	2 2 0 1 2	
3.480E-01	4.389E+01	94.80	C023	2 2 0 1 2	
3.812E-01	4.807E+01	99	C023	2 2 0 1 2	
3.776E-01	4.762E+01	100	M043	1 0 0 0 1	

173. $C_3H_6N_6O_6$

Cyclonite
RDX

RN: 121-82-4 **MP** (°C)**:** 205
MW: 222.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	5.975E-02	25	B173	2 0 2 2 2	

174. C_3H_6O

Propylene oxide
Methyl ethylene oxide

RN: 75-56-9 **MP** (°C)**:** –112
MW: 58.08 **BP** (°C)**:** 34.23

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E+00	2.883E+02	20	I313	0 0 0 0 0	
2.544E-01	1.478E+01	20	M065	1 0 2 1 1	*sic*
6.389E+00	3.711E+02	25	I313	0 0 0 0 0	

175. C_3H_6O

Acetone
2-Propanone
Aceton

RN: 67-64-1 **MP** (°C)**:** –94
MW: 58.08 **BP** (°C)**:** 56.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
		4	C423	0 0 0 0 0	
		10	C423	0 0 0 0 0	

176. C_3H_6O

Propaldehyde
Propyl aldehyde
Propanal

RN: 123-38-6 **MP** (°C)**:** –81
MW: 58.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E+00	1.667E+02	20	D041	1 0 0 0 0	
2.927E+00	1.700E+02	20	F300	1 0 0 0 1	
5.269E+00	3.060E+02	25	A049	1 0 0 0 2	
3.105E+00	1.803E+02	25	B060	2 0 1 1 1	
2.880E+00	1.673E+02	25	F044	1 0 0 0 2	

177. $C_3H_6O_2$

Propionic acid
n-Propionic acid

RN: 79-09-4 **MP** (°C)**:** –22
MW: 74.08 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.025E+01	25	B004	0 0 0 0 0	

178. $C_3H_6O_2$

Ethyl formate
Ameisensaeure-aethyl ester
Formic acid ethyl ester

RN: 109-94-4 **MP** (°C)**:** –80
MW: 74.08 **BP** (°C)**:** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.094E+00	8.108E+01	5.0	K079	1 0 0 0 2	
1.139E+00	8.437E+01	15.9	K079	1 0 0 0 2	
1.350E+00	1.000E+02	18	F300	1 0 0 0 1	
1.350E+00	1.000E+02	22	S006	1 0 0 0 2	
1.194E+00	8.848E+01	30.2	K079	1 0 0 0 2	
1.239E+00	9.178E+01	38.0	K079	1 0 0 0 2	
1.283E+00	9.507E+01	45.1	K079	1 0 0 0 2	
1.339E+00	9.918E+01	50.0	K079	1 0 0 0 2	
1.383E+00	1.025E+02	55.5	K079	1 0 0 0 2	
1.517E+00	1.124E+02	63.9	K079	1 0 0 0 2	
1.639E+00	1.214E+02	70.0	K079	1 0 0 0 2	
1.778E+00	1.317E+02	75.5	K079	1 0 0 0 2	

179. $C_3H_6O_2$

Methyl acetate
Essigsaeures methyl
Methylacetat

RN: 79-20-9 **MP** (°C)**:** –98.0
MW: 74.08 **BP** (°C)**:** 56.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.678E+00	2.725E+02	5.0	K079	1 0 0 0 2	
4.017E+00	2.976E+02	20	E002	1 0 0 0 2	
3.290E+00	2.437E+02	20	F001	1 0 1 2 2	
2.647E+00	1.961E+02	20	F300	1 0 0 0 2	
3.290E+00	2.437E+02	20	M171	1 0 0 0 2	
4.617E+00	3.420E+02	20	P040	0 0 0 0 0	
4.300E+00	3.185E+02	20	S006	1 0 0 0 1	
3.722E+00	2.757E+02	21.0	K079	1 0 0 0 2	
2.772E-02	2.054E+00	25	B004	0 0 0 0 0	*sic*
3.772E+00	2.794E+02	35.0	K079	1 0 0 0 2	
3.889E+00	2.881E+02	58.0	K079	1 0 0 0 2	
3.906E+00	2.893E+02	58.9	K079	1 0 0 0 2	
3.922E+00	2.906E+02	60.1	K079	1 0 0 0 2	
3.950E+00	2.926E+02	61.7	K079	1 0 0 0 2	
4.172E+00	3.091E+02	69.1	K079	1 0 0 0 2	
4.256E+00	3.153E+02	70.5	K079	1 0 0 0 2	
4.294E+00	3.181E+02	71.9	K079	1 0 0 0 2	
4.906E+00	3.634E+02	83.5	K079	1 0 0 0 2	
4.252E-02	3.150E+00	c	L055	0 0 0 0 2	

180. $C_3H_6O_2S_3$
α-Trimethylene trisulphide dioxide
1,3,5-Trithiane, 1,3-dioxide, *trans*-
RN: 60077-04-5 **MP** (°C)**:**
MW: 170.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.817E-02	1.672E+01	25	B112	1 2 1 1 2	

181. $C_3H_6O_2S_3$
β-Trimethylene trisulphide dioxide
1,3,5-Trithiane, 1,3-dioxide, *cis*-
RN: 60041-48-7 **MP** (°C)**:**
MW: 170.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.545E-01	4.334E+01	25	B112	1 2 1 1 2	

182. $C_3H_6O_3$
DL-Glyceraldehyde
DL-Glycerin-aldehyd
RN: 56-82-6 **MP** (°C)**:** 145
MW: 90.08 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E-01	2.913E+01	18	D041	1 0 0 0 0	
3.242E-01	2.920E+01	18	F300	1 0 0 0 2	

183. $C_3H_6O_3$
Hydracrylic acid
Hydracrylsaeure
RN: 503-66-2 **MP** (°C)**:**
MW: 90.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.998E+00	2.701E+02	25	I307	0 0 0 0 0	

184. $C_3H_6O_3$
s-Trioxane
1,3,5-Trioxan
RN: 110-88-3 **MP** (°C)**:** 64
MW: 90.08 **BP** (°C)**:** 114.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E+00	1.544E+02	20.00	B394	0 0 0 0 0	
1.943E+00	1.750E+02	25	F300	1 0 0 0 2	
2.033E+00	1.831E+02	25.00	B394	0 0 0 0 0	
2.403E+00	2.165E+02	30.10	B394	0 0 0 0 0	
2.741E+00	2.469E+02	34.45	B394	0 0 0 0 0	
4.187E+00	3.772E+02	43.00	B394	0 0 0 0 0	
4.462E+00	4.019E+02	44.00	B394	0 0 0 0 0	
4.606E+00	4.149E+02	44.40	B394	0 0 0 0 0	
4.826E+00	4.348E+02	45.00	B394	0 0 0 0 0	
4.816E+00	4.338E+02	45.10	B394	0 0 0 0 0	
5.355E+00	4.824E+02	46.00	B394	0 0 0 0 0	
5.311E+00	4.784E+02	46.10	B394	0 0 0 0 0	
6.401E+00	5.766E+02	47.10	B394	0 0 0 0 0	
8.161E+00	7.351E+02	47.80	B394	0 0 0 0 0	
8.534E+00	7.687E+02	48.95	B394	0 0 0 0 0	
8.741E+00	7.874E+02	50.20	B394	0 0 0 0 0	
9.095E+00	8.192E+02	55.30	B394	0 0 0 0 0	

185. $C_3H_6O_3S_3$
α-Trimethylene trisulphoxide
1,3,5-Trithiane, 1,3,5-trioxide, (1α,3α,5α)-
RN: 60102-87-6 **MP** (°C)**:**
MW: 186.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.184E-03	1.338E+00	25	B112	1 2 1 1 2	

186. $C_3H_6O_3S_3$
β-Trimethylene trisulphoxide
1,3,5-Trithiane, 1,3,5-trioxide, (1α,3α,5β)-
RN: 60102-88-7 **MP** (°C)**:**
MW: 186.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-02	1.417E+01	25	B112	1 2 1 1 2	

187. $C_3H_6O_3S$
1,3-Propane sultone
1,2-Oxathiolane 2,2-dioxide
3-Hydroxy-1-propanesulfonic acid g-sultone
RN: 1120-71-4 **MP** (°C)**:** 31
MW: 122.14 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.187E-01	1.000E+02	ns	I307	0 0 0 0 0	

188. C_3H_7Br
Isopropyl bromide
Isopropylbromid
RN: 75-26-3 **MP** (°C)**:** –89
MW: 123.00 **BP** (°C)**:** 59

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-02	4.180E+00	0	H101	2 0 0 0 2	
2.340E-02	2.878E+00	18	F001	1 0 1 2 2	
2.602E-02	3.200E+00	20	F300	1 0 0 0 1	
2.585E-02	3.180E+00	20	H101	2 0 0 0 2	
2.592E-02	3.188E+00	30	V009	1 0 0 0 1	

189. C_3H_7Br
Propyl bromide
1-Bromopropane
Propylbromid
Bromopropane
RN: 106-94-5 **MP** (°C)**:** –110
MW: 123.00 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-02	2.970E+00	0	F300	1 0 0 0 2	
2.423E-02	2.980E+00	0	H101	2 0 0 0 2	
1.850E-02	2.275E+00	19.5	S006	1 0 0 0 2	
1.850E-02	2.275E+00	19.50	F001	1 0 1 0 2	
1.992E-02	2.450E+00	20	H101	2 0 0 0 2	
1.947E-02	2.394E+00	20	H127	1 0 0 0 1	
1.874E-02	2.305E+00	30	G029	1 0 2 2 2	
1.876E-02	2.307E+00	30	V009	1 0 0 0 2	
1.140E-01	1.402E+01	ns	H307	0 0 0 0 0	

190. C_3H_7BrO
3-Bromo-1-propanol
3-Brom-propanol-(1)
RN: 627-18-9 **MP** (°C)**:**
MW: 139.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.022E+00	1.420E+02	20	F300	1 0 0 0 2	

191. C_3H_7Cl
Isopropyl chloride
2-Chloropropane
RN: 75-29-6 **MP** (°C)**:** –117
MW: 78.54 **BP** (°C)**:** 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.602E-02	4.400E+00	0	H101	2 0 0 0 2	
4.380E-02	3.440E+00	12.50	F001	1 0 1 0 2	
3.947E-02	3.100E+00	20	F300	1 0 0 0 1	
3.883E-02	3.050E+00	20	H101	2 0 0 0 2	
3.935E-02	3.090E+00	20	N034	1 0 0 0 1	
3.888E-02	3.054E+00	30	V009	1 0 0 0 1	

192. C_3H_7Cl
Chloropropane
Propyl chloride
1-Chloropropane
RN: 540-54-5 **MP** (°C)**:** –123
MW: 78.54 **BP** (°C)**:** 43.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.787E-02	3.760E+00	0	H101	2 0 0 0 2	
2.970E-02	2.333E+00	12.50	F001	1 0 1 0 2	
3.438E-02	2.700E+00	20	F300	1 0 0 0 1	
3.463E-02	2.720E+00	20	H101	2 0 0 0 2	
3.428E-02	2.693E+00	20	N034	1 0 0 0 1	
2.970E-02	2.333E+00	20	S006	1 0 0 0 2	
3.520E-02	2.765E+00	30	V009	1 0 0 0 2	

193. C_3H_7ClO

3-Chloro-1-propanol
3-Chlor-propanol-(1)
RN: 627-30-5 **MP** (°C)**:**
MW: 94.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E+00	2.500E+02	20	F300	1 0 0 0 1	
+2.64E+00	+2.50E+02	ns	S460	0 0 0 0 0	

194. C_3H_7I

Iodopropane
n-Propyl iodide
RN: 107-08-4 **MP** (°C)**:** –101
MW: 169.99 **BP** (°C)**:** 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-03	1.140E+00	0	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	F001	1 0 1 0 2	
5.118E-03	8.700E-01	20	F300	1 0 0 0 1	
6.294E-03	1.070E+00	20	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	M171	1 0 0 0 1	
5.100E-03	8.670E-01	20	S006	1 0 0 0 1	
6.258E-03	1.064E+00	23.5	S171	2 1 2 2 2	
6.112E-03	1.039E+00	30	G029	1 0 2 2 2	
6.094E-03	1.036E+00	30	V009	1 0 0 0 1	

195. C_3H_7I

Isopropyl iodide
2-Iodopropane
RN: 75-30-9 **MP** (°C)**:** –90
MW: 169.99 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.824E-03	1.670E+00	0	H101	2 0 0 0 2	
8.236E-03	1.400E+00	20	F300	1 0 0 0 1	
8.236E-03	1.400E+00	20	H101	2 0 0 0 2	
7.889E-03	1.341E+00	30	V009	1 0 0 0 1	

196. $C_3H_7NO_2$

1-Nitropropane
n-Nitropropane

RN: 108-03-2 **MP** (°C)**:** –108
MW: 89.09 **BP** (°C)**:** 131.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-01	1.381E+01	20	C121	1 0 0 0 1	unit assumed, *sic*

197. $C_3H_7NO_2$

2-Nitropropane
Nitroisopropane
Dimethylnitromethane

RN: 79-46-9 **MP** (°C)**:** –93
MW: 89.09 **BP** (°C)**:** 120.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-01	1.672E+01	20	C121	0 0 0 0 1	unit assumed, *sic*
1.874E-01	1.670E+01	20	F300	1 0 0 0 2	
2.376E-01	2.117E+01	20	H118	1 1 1 1 2	

198. $C_3H_7NO_2$

α-Alanine
Alanine
2-Aminopropanoic acid
2-Ammoniopropanoate
L-2-Aminopropionic acid

RN: 56-41-7 **MP** (°C)**:** 314.5–316.5
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E+00	1.217E+02	10	C347	0 0 0 0 0	EFG
1.640E+00	1.461E+02	15	D349	2 1 1 2 2	
1.744E+00	1.554E+02	20	B032	1 2 2 1 2	
1.535E+00	1.367E+02	20	C347	0 0 0 0 0	EFG
1.780E+00	1.586E+02	20	D349	2 1 1 2 2	
1.838E+00	1.638E+02	25	B032	1 2 2 1 2	
1.590E+00	1.417E+02	25	D005	2 2 1 1 2	
1.602E+00	1.427E+02	25	D041	1 0 0 0 2	
1.870E+00	1.666E+02	25	D349	2 1 1 2 2	
1.660E+00	1.479E+02	25	E015	1 2 1 1 1	
1.595E+00	1.421E+02	25	G092	2 1 1 1 1	
1.595E+00	1.421E+02	25	G315	0 0 0 0 0	
1.654E+00	1.474E+02	25	G433	0 0 0 0 0	
1.852E+00	1.650E+02	25	J303	0 0 0 0 0	
1.600E+00	1.426E+02	25	N001	0 0 0 0 0	EFG
1.630E+00	1.452E+02	25	N012	2 0 2 1 2	
1.555E+00	1.386E+02	25	O316	1 0 1 2 2	

(*continued*)

198. $C_3H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.598E+00	1.424E+02	25	O316	1 0 1 2 2	
1.623E+00	1.446E+02	25	O317	1 0 1 2 2	
1.871E+00	1.667E+02	25.1	N024	0 0 0 0 0	
1.871E+00	1.667E+02	25.1	N026	0 0 0 0 0	
1.606E+00	1.431E+02	25.1	N027	1 1 2 2 2	
1.704E+00	1.518E+02	27	D036	0 0 0 0 0	
1.695E+00	1.510E+02	27	D036	0 0 0 0 0	
1.940E+00	1.728E+02	29.80	B032	1 2 2 1 2	
1.657E+00	1.477E+02	30	C347	0 0 0 0 0	EFG
1.956E+00	1.743E+02	30	J303	0 0 0 0 0	
1.816E+00	1.618E+02	40	C347	0 0 0 0 0	EFG
2.192E+00	1.953E+02	40	J303	0 0 0 0 0	
1.931E+00	1.720E+02	45	F300	1 0 0 0 2	
1.932E+00	1.721E+02	50	C347	0 0 0 0 0	EFG
2.430E+00	2.165E+02	50	J303	0 0 0 0 0	
2.118E+00	1.887E+02	60	C347	0 0 0 0 0	EFG
2.706E+00	2.411E+02	60	J303	0 0 0 0 0	
2.333E+00	2.078E+02	70	C347	0 0 0 0 0	EFG
2.489E+00	2.218E+02	75	D041	1 0 0 0 2	
2.504E+00	2.230E+02	80	C347	0 0 0 0 0	EFG
2.668E+00	2.377E+02	90	C347	0 0 0 0 0	EFG
2.888E+00	2.573E+02	100	C347	0 0 0 0 0	EFG
1.192E+00	1.062E+02	-	C347	0 0 0 0 0	EFG
1.587E+00	1.414E+02	rt	D021	0 0 1 1 2	

199. $C_3H_7NO_2$

β-Alanine
β-Alanin
RN: 107-95-9 **MP** (°C)**:**
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E+00	3.528E+02	25	D041	1 0 0 0 2	
6.123E+00	5.455E+02	25	M024	1 2 0 1 2	

200. $C_3H_7NO_2$

D-Alanine
D(–)-Alanine
RN: 338-69-2 **MP** (°C)**:** 292
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E+00	1.127E+02	0	M043	1 0 0 0 2	
1.396E+00	1.243E+02	10	M043	1 0 0 0 2	

(*continued*)

200. $C_3H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E+00	1.363E+02	20	D041	1 0 0 0 2	
1.531E+00	1.364E+02	20	M043	1 0 0 0 2	
1.589E+00	1.416E+02	25	D005	2 2 1 1 2	
1.680E+00	1.497E+02	30	M043	1 0 0 0 2	
1.839E+00	1.639E+02	40	M043	1 0 0 0 2	
2.194E+00	1.955E+02	60	M043	1 0 0 0 2	
2.590E+00	2.308E+02	80	M043	1 0 0 0 2	
3.049E+00	2.717E+02	100	M043	1 0 0 0 2	
3.049E+00	2.717E+02	99.99	P349	0 0 0 0 0	

201. $C_3H_7NO_2$

DL-Alanine
DL-α-Alanine
DL-2-Aminopropionic acid

RN: 302-72-7 **MP** (°C)**:** 289
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	1.080E+02	0	D018	2 2 2 1 2	
1.212E+00	1.080E+02	0	F300	1 0 0 0 2	
1.212E+00	1.079E+02	0	M043	1 0 0 0 2	
1.361E+00	1.213E+02	10	M043	1 0 0 0 0	
1.523E+00	1.357E+02	20	M043	1 0 0 0 0	
1.557E+00	1.387E+02	21	P045	1 0 2 1 2	
1.659E+00	1.478E+02	25	C018	0 0 0 0 0	
1.596E+00	1.422E+02	25	D018	2 2 2 1 2	
1.598E+00	1.424E+02	25	D041	1 0 0 0 2	
1.607E+00	1.432E+02	25	F300	1 0 0 0 2	
1.900E+00	1.693E+02	25	J303	0 0 0 0 0	
1.530E+00	1.363E+02	25	K031	2 1 2 1 2	
2.024E+00	1.803E+02	30	J303	0 0 0 0 0	
1.704E+00	1.518E+02	30	M043	1 0 0 0 0	
2.307E+00	2.055E+02	40	J303	0 0 0 0 0	
1.894E+00	1.687E+02	40	M043	1 0 0 0 0	
2.134E+00	1.902E+02	50	D018	2 2 2 1 2	
2.106E+00	1.876E+02	50	F300	1 0 0 0 2	
2.591E+00	2.308E+02	50	J303	0 0 0 0 0	
2.954E+00	2.632E+02	60	J303	0 0 0 0 0	
2.337E+00	2.082E+02	60	M043	1 0 0 0 0	
2.733E+00	2.435E+02	75	D018	2 2 2 1 2	
2.734E+00	2.436E+02	75	D041	1 0 0 0 2	
2.714E+00	2.418E+02	75	F300	1 0 0 0 2	
2.842E+00	2.532E+02	80	M043	1 0 0 0 0	
3.431E+00	3.057E+02	100	F300	1 0 0 0 2	
3.430E+00	3.056E+02	100	M043	1 0 0 0 2	
3.432E+00	3.057E+02	99.99	P349	0 0 0 0 0	

202. $C_3H_7NO_2$
Lactamide
2-Hydroxypropionamide
RN: 2043-43-8 **MP** (°C)**:**
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.779E+00	7.822E+02	25	M008	1 0 0 0 2	

203. $C_3H_7NO_2$
Sarcosine
Sarkosin
RN: 107-97-1 **MP** (°C)**:** 208
MW: 89.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.151E-01	4.589E+01	20	D041	1 0 0 0 2	
3.367E+00	3.000E+02	20	F300	1 0 0 0 2	
4.807E+00	4.282E+02	20	P045	1 0 2 1 2	

204. $C_3H_7NO_2$
Urethan
Carbamidsaeure-aethyl ester
Eythyl urethan
Urethane
Ethyl carbamate
Carbamic acid ethyl ester
RN: 51-79-6 **MP** (°C)**:** 49
MW: 89.09 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E+00	2.600E+02	11	F300	1 0 0 0 1	
5.393E+00	4.805E+02	15.5	F001	1 0 1 2 2	
2.245E+01	2.000E+03	25	I310	0 0 0 0 0	
5.074E+00	4.521E+02	25	P065	2 0 1 1 2	
1.800E+01	1.604E+03	37	H006	1 2 2 1 1	
8.901E+00	7.930E+02	40	F300	1 0 0 0 2	

205. $C_3H_7NO_2S$
Cysteine
2-Amino-3-mercaptopropanoic acid
RN: 3374-22-9 **MP** (°C)**:** 225
MW: 121.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.773E-02	3.360E+00	20	P045	1 0 2 1 2	

206. $C_3H_7NO_3$
Serine
2-Amino-3-hydroxypropanoic acid
L(–)-Serin
RN: 56-45-1 **MP** (°C)**:** 220
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.556E+00	1.635E+02	10.19	J417	0 0 0 0 0	
1.626E+00	1.709E+02	12.69	J417	0 0 0 0 0	
4.530E-01	4.761E+01	15	D349	2 1 1 2 2	
1.864E+00	1.959E+02	16.09	J417	0 0 0 0 0	
1.903E+00	2.000E+02	20	D041	1 0 0 0 1	
4.610E-01	4.845E+01	20	D349	2 1 1 2 2	
9.512E-01	9.997E+01	20	F300	1 0 0 0 2	
3.405E+00	3.578E+02	20.00	B032	1 2 2 1 2	*sic*
4.700E-01	4.939E+01	25	D349	2 1 1 2 2	
2.807E+00	2.950E+02	25	G315	0 0 0 0 0	*sic*
4.013E+00	4.217E+02	25	J303	0 0 0 0 0	
4.043E+00	4.249E+02	25.00	B032	1 2 2 0 2	*sic*
2.228E+00	2.342E+02	25.89	J417	0 0 0 0 0	
3.578E+00	3.760E+02	27	D036	0 0 0 0 0	
2.287E+00	2.404E+02	27.89	J417	0 0 0 0 0	
4.690E+00	4.929E+02	29.80	B032	1 2 2 1 2	*sic*
5.633E+00	5.920E+02	40	J303	0 0 0 0 0	
2.800E+00	2.943E+02	42.79	J417	0 0 0 0 0	
2.811E+00	2.954E+02	43.79	J417	0 0 0 0 0	
2.861E+00	3.007E+02	44.59	J417	0 0 0 0 0	
2.902E+00	3.050E+02	49.69	J417	0 0 0 0 0	
2.972E+00	3.124E+02	53.89	J417	0 0 0 0 0	
7.574E+00	7.960E+02	60	J303	0 0 0 0 0	

207. $C_3H_7NO_3$
D-Serine
D-2-Amino-3-hydroxypropanoic acid
RN: 312-84-5 **MP** (°C)**:** 220
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.903E+00	2.000E+02	20	D041	1 0 0 0 0	
4.010E+00	4.214E+02	25	J303	0 0 0 0 0	
5.709E+00	6.000E+02	40	J303	0 0 0 0 0	
7.631E+00	8.020E+02	60	J303	0 0 0 0 0	

208. $C_3H_7NO_3$

DL-Serine
DL-2-Amino-3-hydroxypropanoic acid
RN: 302-84-1 **MP** (°C)**:** 240
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-01	2.920E+01	10	F300	1 0 0 0 2	
3.787E-01	3.980E+01	20	F300	1 0 0 0 2	
4.548E-01	4.780E+01	25	D041	1 0 0 0 2	
4.805E-01	5.050E+01	25	J303	0 0 0 0 0	
7.403E-01	7.780E+01	40	J303	0 0 0 0 0	
8.916E-01	9.370E+01	50	F300	1 0 0 0 2	
1.261E+00	1.325E+02	60	J303	0 0 0 0 0	
1.533E+00	1.611E+02	75	D041	1 0 0 0 2	
1.532E+00	1.610E+02	75	F300	1 0 0 0 2	
2.320E+00	2.438E+02	100	F300	1 0 0 0 2	
2.320E+00	2.438E+02	99.99	P349	0 0 0 0 0	

209. $C_3H_7NO_3$

DL-Isoserine
DL-Isoserin
RN: 632-12-2 **MP** (°C)**:** 235
MW: 105.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	1.530E+01	20	F300	1 0 0 0 2	

210. $C_3H_7NO_5$

Glycerol-α-nitrate
Glycerin-α-nitrate
RN: 27321-61-5 **MP** (°C)**:**
MW: 137.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E+00	4.118E+02	15	F300	1 0 0 0 2	

211. $C_3H_7N_3O_2$

Glycocyamine
Guanidin-essigsaeure
Guanidineacetic acid
RN: 352-97-6 **MP** (°C)**:** 280
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-02	4.480E+00	15	D041	1 0 0 0 1	
3.074E-02	3.600E+00	15	F300	1 0 0 0 1	

212. $C_3H_7N_3O_2$
Nitrosoethylurea
N-Nitroso-*N*-ethylurea
RN: 759-73-9 **MP** (°C)**:** 103
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	1.283E+01	rt	I306	0 0 0 0 0	

213. $C_3H_7O_5P$
2-Carboxyethylphosphonic acid
3-Phosphonopropionic acid
RN: 5962-42-5 **MP** (°C)**:**
MW: 154.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	2.842E+02	0	N028	1 0 0 0 2	
2.129E+00	3.280E+02	20	N028	1 0 0 0 2	

214. C_3H_8
Propane
Propan
RN: 74-98-6 **MP** (°C)**:** –187
MW: 44.10 **BP** (°C)**:** –42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.460E-03	1.526E-01	4	K031	2 1 2 1 2	
2.472E-03	1.090E-01	10	F300	1 0 0 0 2	
2.721E-03	1.200E-01	18	M065	0 0 2 1 1	1 atm, *sic*
1.761E-03	7.765E-02	19.8	G058	1 0 0 0 2	
1.746E-03	7.700E-02	20	F300	1 0 0 0 1	
1.420E-03	6.261E-02	25	B342	1 2 1 1 1	
1.530E-03	6.747E-02	25	K031	2 1 2 1 2	
1.415E-03	6.240E-02	25	M001	2 1 2 2 2	
1.415E-03	6.240E-02	25	M002	2 1 2 2 2	
8.400E-04	3.704E-02	50	K031	2 1 2 1 2	
6.123E-04	2.700E-02	60	F300	1 0 0 0 1	

215. $C_3H_8NO_5P$

Glyphosate
N-(Phosphonomethyl)glycine
Bronco
RN: 1071-83-6 **MP** (°C)**:** 230.0
MW: 169.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.097E-02	1.200E+01	25	M161	1 0 0 0 1	
5.856E-02	9.901E+00	ns	B100	0 0 0 0 0	

216. C_3H_8O

n-Propyl alcohol
Propanol
RN: 71-23-8 **MP** (°C)**:** –127.0
MW: 60.10 **BP** (°C)**:** 97.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E+00	1.882E+02	ns	L003	0 0 2 1 2	
+4.17E+00	+2.51E+02	ns	S460	0 0 0 0 0	

217. C_3H_8O

Isopropyl alcohol
2-Propanol
RN: 67-63-0 **MP** (°C)**:** –88
MW: 60.10 **BP** (°C)**:** 82.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.033E+00	3.025E+02	ns	L003	0 0 2 1 1	

218. $C_3H_8OS_2$

2,3-Dimercapto-1-propanol
Dimercaprol
RN: 59-52-9 **MP** (°C)**:**
MW: 124.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.963E-01	7.407E+01	20	D041	1 0 0 0 0	

219. $C_3H_8O_2$
Methylal
Formaldehyd-dimethyl-acetal
RN: 109-87-5 **MP** (°C)**:** –105
MW: 76.10 **BP** (°C)**:** 41.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E+00	2.441E+02	16	B117	1 0 0 1 2	
3.022E+00	2.300E+02	20	F300	1 0 0 0 1	

220. $C_3H_8O_3$
Glycerol
Glycerin
RN: 56-81-5 **MP** (°C)**:** 20
MW: 92.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.973E+00	5.501E+02	4.50	C022	1 2 0 0 2	
5.751E-01	5.296E+01	25	B004	0 0 0 0 0	

221. C_3H_9N
Propylamine
Propylamin
n-Propylamine
RN: 107-10-8 **MP** (°C)**:** –83
MW: 59.11 **BP** (°C)**:** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	1.459E+00	25	B004	0 0 0 0 0	

222. C_3H_9N
Trimethylamine
N,*N*-Dimethylmethanamine
RN: 75-50-3 **MP** (°C)**:** –124.0
MW: 59.11 **BP** (°C)**:** 3.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.77E+00	>4.00E+02	20	F300	1 0 0 0 0	
6.936E+00	4.100E+02	25	A049	1 0 0 0 2	

223. $C_3H_9O_4P$
Trimethyl phosphate
Phosphorsaeure-trimethyl ester
RN: 512-56-1 **MP** (°C)**:**
MW: 140.08 **BP** (°C)**:** 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E+00	5.000E+02	25	F300	1 0 0 0 1	
3.573E+00	5.005E+02	ns	S460	0 0 0 0 0	

224. $C_3H_{12}N_6O_3$
Guanidine carbonate
Guanidin-carbonat
RN: 3425-08-9 **MP** (°C)**:** 198
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E+00	3.333E+02	24	F300	1 0 0 0 2	

225. $C_3Cl_3N_3O_3$
Trichloroisocyanuric acid
Symclosene
RN: 87-90-1 **MP** (°C)**:** 246.5
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.439E-03	7.994E-01	20	B080	1 0 1 1 0	
2.311E-02	5.371E+00	40	B080	1 0 1 1 1	

226. C_3Cl_6
Hexachloropropene
Hexachloropropylene
Perchloropropene
Hexachloro-1-propene
1,1,2,3,3,3-Hexachloro-1-propene
1,1,2,3,3,3-Hexachloropropene
RN: 1888-71-7 **MP** (°C)**:**
MW: 248.75 **BP** (°C)**:** 209–210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.026E-04	1.499E-01	ns	S460	0 0 0 0 0	

227. C_4HI_4N
Iodol
2,3,4,5-Tetraiodpyrrol
RN: 87-58-1 **MP** (°C)**:**
MW: 570.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.505E-04	2.000E-01	15	F300	1 0 0 0 2	

228. C_4H_2
Butadiyne
Diacetylen
RN: 460-12-8 **MP** (°C)**:** –36.4
MW: 50.06 **BP** (°C)**:** 10.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	1.000E-01	25	F300	1 0 0 0 0	

229. $C_4H_2N_2O_4$
Alloxan
Alloxane
RN: 50-71-5 **MP** (°C)**:** 256dec
MW: 142.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.631E-02	8.000E+00	ns	D072	0 0 0 0 0	
5.623E-02	7.989E+00	ns	R424	0 0 0 0 0	

230. $C_4H_3BrN_2O_2$
5-Bromouracil
5-Bromo-2
4(1H,3H)-Pyrimidinedione
5-Bromo-2,4-dihydroxypyrimidine
Bromouracil
RN: 51-20-7 **MP** (°C)**:** 310
MW: 190.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.507E-02	2.878E+00	25	S471	0 0 0 0 0	
1.908E-02	3.644E+00	25	S471	0 0 0 0 0	
1.350E-02	2.578E+00	25	Z408	0 0 0 0 0	

231. $C_4H_3ClN_2O_2$

6-Chlorouracil
4-Chloro-2,6-dihydroxypyrimidine
RN: 4270-27-3 **MP** (°C)**:**
MW: 146.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.334E-02	4.885E+00	25	S471	0 0 0 0 0	
3.350E-02	4.909E+00	25	S471	0 0 0 0 0	

232. $C_4H_3ClN_2O_2$

5-Chlorouracil
RN: 1820-81-1 **MP** (°C)**:**
MW: 146.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.707E-02	2.501E+00	25	S471	0 0 0 0 0	
1.712E-02	2.509E+00	25	S471	0 0 0 0 0	
1.800E-02	2.638E+00	25	Z408	0 0 0 0 0	
9.827E-04	1.440E-01	ns	Y414	0 0 0 0 0	

233. $C_4H_3FN_2O_2$

5 Fluorouracil
5-Fluorouracil
Fluorouracil
5-Fluoro-2,4(1H,3H)-pyrimidinedione
Fluroblastin
Fluororuracil
RN: 51-21-8 **MP** (°C)**:** 281
MW: 130.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-02	1.249E+01	21	B416	2 2 1 2 1	
8.533E-02	1.110E+01	22	B321	0 0 0 0 0	pH 4.0
8.533E-02	1.110E+01	22	B332	1 1 0 0 1	pH 4.0
8.533E-02	1.110E+01	22	B388	0 0 0 0 0	
9.379E-02	1.220E+01	22	M317	1 1 1 1 1	
9.379E-02	1.220E+01	25	R023	0 0 0 0 0	
1.356E-01	1.763E+01	25	S471	0 0 0 0 0	
1.382E-01	1.798E+01	25	S471	0 0 0 0 0	
6.940E-02	9.027E+00	25	Z408	0 0 0 0 0	
8.533E-02	1.110E+01	37	B332	0 0 0 0 0	pH 4.0
9.566E-02	1.244E+01	ns	S469	0 0 0 0 0	

234. $C_4H_3IN_2O_2$

5-Iodouracil
5-Iodo-2,4(1H,3H)-pyrimidinedione
5-Iodo-2,4-dihydroxypyrimidine

RN: 696-07-1 **MP** (°C)**:** 274–276 (°dec)
MW: 237.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-02	4.907E+00	25	S471	0 0 0 0 0	
2.072E-02	4.931E+00	25	S471	0 0 0 0 0	
1.060E-02	2.523E+00	25	Z408	0 0 0 0 0	

235. $C_4H_3N_2S$

2-Methyl-1,3,4-thiadiazole
Thiodiazolique methyle

RN: 26584-42-9 **MP** (°C)**:**
MW: 111.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.918E-03	8.800E-01	37	D084	1 0 1 0 1	

236. $C_4H_3N_3O_4$

5-Nitrouracil

RN: 611-08-5 **MP** (°C)**:**
MW: 157.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	3.613E+00	25	Z408	0 0 0 0 0	

237. $C_4H_3N_3O_5$

5-Nitrobarbituric acid
Dilitursaeure

RN: 28176-10-5 **MP** (°C)**:** 176
MW: 173.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	9.000E-01	25.60	F300	1 0 0 0 0	

238. $C_4H_4Br_2O_4$

meso-2,3-Dibromosuccinic acid
meso-Dibrom-bernsteinsaeure
DL-2,3-Dibromosuccinic acid
DL-Dibrom-bernsteinsaeure

RN: 526-78-3 **MP** (°C)**:** 171
MW: 275.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.249E-02	2.000E+01	17	F300	1 0 0 0 2	

239. $C_4H_4Cl_2N_2O_2$

1,3-Dichloro-5-methylhydantoin
2,4-Imidazolidinedione, 1,3-dichloro-5-methyl-
Hydantoin, 1,3-dichloro-5-methyl-

RN: 15216-12-3 **MP** (°C)**:**
MW: 182.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.634E-02	2.991E+00	20	B080	1 0 1 1 0	
4.498E-02	8.232E+00	40	B080	1 0 1 1 1	

240. $C_4H_4Cl_2O_4$

L-2,3-Dichlorosuccinic acid
L(–)-Dichlor-bernsteinsaeure
D-2,3-Dichlorosuccinic acid
D(+)-Dichlor-bernsteinsaeure
2,3-Dichlorosuccinic acid
meso-2,3-Dichlorosuccinic acid

RN: 19922-87-3 **MP** (°C)**:** 168
MW: 186.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.674E+00	5.000E+02	25	H090	0 1 1 1 1	
1.701E-02	3.180E+00	ns	H090	0 2 2 1 2	

241. $C_4H_4N_2$

Succinonitrile
Bersteinsaeure-dinitril

RN: 110-61-2 **MP** (°C)**:** 57
MW: 80.09 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E+00	1.269E+02	20	F300	1 0 0 0 2	

242. $C_4H_4N_2O$
4(3H)-Pyrimidone
4-Hydroxypyrimidine
RN: 51953-17-4 **MP** (°C)**:** 164
MW: 96.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E+00	2.703E+02	20	B050	1 0 0 0 0	

243. $C_4H_4N_2O$
2-Hydroxypyrimidine
2-Pyrimidinol
RN: 51953-13-0 **MP** (°C)**:**
MW: 96.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.252E+00	3.125E+02	20	B050	1 0 0 0 0	

244. $C_4H_4N_2OS$
2-Thiouracil
Thiouracil
4(1H)-Pyrimidinone
RN: 141-90-2 **MP** (°C)**:** 340
MW: 128.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-03	5.996E-01	20	D041	1 0 0 0 0	
5.530E-03	7.087E-01	25	G016	1 2 1 2 2	intrinsic
3.900E-03	4.998E-01	ns	I310	0 0 0 0 0	

245. $C_4H_4N_2O_2$
Uracil
2,4-Dihydroxypyrimidine
RN: 66-22-8 **MP** (°C)**:** 335
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	
2.500E-02	2.802E+00	20	N019	0 0 0 0 0	
3.200E-02	3.587E+00	25	D041	1 0 0 0 1	
3.212E-02	3.600E+00	25	F300	1 0 0 0 1	
2.380E-02	2.668E+00	25	H061	0 0 0 0 0	
4.109E-02	4.605E+00	25	S471	0 0 0 0 0	
4.125E-02	4.624E+00	25	S471	0 0 0 0 0	

(*continued*)

245. $C_4H_4N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-02	3.038E+00	25	Z408	0 0 0 0 0	
4.015E-02	4.500E+00	37	B390	0 0 0 0 0	
2.676E-02	3.000E+00	ns	B177	0 0 0 0 0	

246. $C_4H_4N_2O_2$

4,6-Dihydroxypyrimidine
4,6-Pyrimidinediol
RN: 1193-24-4 **MP** (°C)**:** >300
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.225E-02	2.494E+00	20	B050	1 0 0 0 0	

247. $C_4H_4N_2O_2$

2,4-Dihydroxypyrimidine
RN: 51953-14-1 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	

248. $C_4H_4N_2O_2$

Maleic hydrazide
Dihydropyridazine-3,6-dione
RN: 123-33-1 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.554E-02	3.984E+00	20	B185	0 0 0 0 0	
5.321E-02	5.964E+00	25	B185	0 0 0 0 0	
5.353E-02	6.000E+00	25	B200	1 0 0 0 2	
5.321E-02	5.964E+00	25	M061	1 0 0 0 0	
5.353E-02	6.000E+00	25	M161	1 0 0 0 0	
5.321E-02	5.964E+00	ns	B100	0 0 0 0 0	
6.310E-03	7.072E-01	ns	M163	0 0 0 0 0	EFG
3.554E-02	3.984E+00	ns	N013	0 0 0 0 0	

249. $C_4H_4N_2O_3$
Barbituric acid
Barbitursaeure
RN: 67-52-7 **MP** (°C)**:** 248
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-07	1.900E-05	37	B166	1 0 1 1 1	
5.129E-02	6.569E+00	ns	R424	0 0 0 0 0	
5.129E-02	6.569E+00	ns	R427	0 0 0 0 0	

250. $C_4H_4N_2O_3$
2,4,6-Trihydroxypyrimidine
2,4,6-Pyrimidinetriol
RN: 223674-01-9 **MP** (°C)**:**
MW: 128.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.170E-02	6.623E+00	20	B050	1 0 0 0 0	

251. $C_4H_4O_4$
trans-Fumaric acid
Fumaric acid
Fumarsaeure
RN: 110-17-8 **MP** (°C)**:** 287
MW: 116.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-02	2.295E+00	0	M043	1 0 0 0 1	
3.005E-02	3.488E+00	10	M043	1 0 0 0 1	
4.286E-02	4.975E+00	20	M043	1 0 0 0 1	
5.989E-02	6.951E+00	25	D041	1 0 0 0 1	
6.031E-02	7.000E+00	25	F300	1 0 0 0 0	
5.989E-02	6.951E+00	25	W011	1 2 2 1 1	
6.159E-02	7.149E+00	30	M043	1 0 0 0 1	
9.218E-02	1.070E+01	40	F300	1 0 0 0 2	
9.374E-02	1.088E+01	40	M043	1 0 0 0 1	
9.121E-02	1.059E+01	40	W011	1 2 2 1 2	
1.937E-01	2.248E+01	60	M043	1 0 0 0 1	
2.019E-01	2.344E+01	60	W011	1 2 2 1 1	
4.258E-01	4.943E+01	80	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	D041	1 0 0 0 1	
8.012E-01	9.300E+01	100	F300	1 0 0 0 1	
7.689E-01	8.925E+01	100	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	W011	1 2 2 1 1	
5.248E-02	6.092E+00	ns	R424	0 0 0 0 0	

252. $C_4H_4O_4$

Maleic acid
Maleinsaeure

RN: 110-16-7 **MP** (°C)**:** 138
MW: 116.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.431E+00	2.821E+02	0	M043	1 0 0 0 2	
2.607E+00	3.026E+02	4.99	A339	0 0 0 0 0	
2.872E+00	3.334E+02	10	F300	1 0 0 0 2	
2.872E+00	3.333E+02	10	M043	1 0 0 0 1	
2.880E+00	3.343E+02	9.99	A339	0 0 0 0 0	
3.094E+00	3.591E+02	14.99	A339	0 0 0 0 0	
3.312E+00	3.845E+02	19.99	A339	0 0 0 0 0	
3.547E+00	4.118E+02	20	M043	1 0 0 0 1	
6.789E+00	7.880E+02	22.5	G301	0 0 0 0 0	
3.592E+00	4.170E+02	24.99	A339	0 0 0 0 0	
3.797E+00	4.407E+02	25	D041	1 0 0 0 2	
3.797E+00	4.407E+02	25	F300	1 0 0 0 2	
3.840E+00	4.457E+02	25	H430	0 0 0 0 0	
3.797E+00	4.407E+02	25	W011	1 2 2 1 2	
3.823E+00	4.437E+02	29.99	A339	0 0 0 0 0	
4.081E+00	4.737E+02	30	M043	1 0 0 0 1	
4.117E+00	4.778E+02	34.99	A339	0 0 0 0 0	
4.300E+00	4.991E+02	39.99	A339	0 0 0 0 0	
4.608E+00	5.349E+02	40	M043	1 0 0 0 2	
4.561E+00	5.294E+02	40	W011	1 2 2 1 2	
4.562E+00	5.295E+02	44.99	A339	0 0 0 0 0	
4.677E+00	5.429E+02	49.99	A339	0 0 0 0 0	
4.842E+00	5.620E+02	54.99	A339	0 0 0 0 0	
5.031E+00	5.840E+02	59.99	A339	0 0 0 0 0	
5.516E+00	6.403E+02	60	M043	1 0 0 0 2	
5.151E+00	5.979E+02	60	W011	1 2 2 1 2	
5.166E+00	5.997E+02	64.99	A339	0 0 0 0 0	
6.366E+00	7.389E+02	80	M043	1 0 0 0 2	
6.864E+00	7.967E+02	97.5	D041	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	F300	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	W011	1 2 2 1 2	

253. C_4H_4S

Thiophene
Thiofuran
Thiacyclopentadiene

RN: 110-02-1 **MP** (°C)**:** –38.3
MW: 84.14 **BP** (°C)**:** 84.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-02	3.015E+00	25	K119	1 0 0 0 2	
3.583E-02	3.015E+00	25	P051	2 1 1 2 2	
3.583E-02	3.015E+00	25.00	P007	2 1 2 2 2	

254. $C_4H_5BrO_4$
Bromosuccinic acid
DL-Brombernsteinsaeure
RN: 923-06-8 **MP** (°C)**:**
MW: 196.99 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.092E-01	1.200E+02	15.5	F300	1 0 0 0 1	

255. $C_4H_5ClO_2$
2-Chloroisocrotonic acid
α-Chlor-isocrotonsaeure
RN: 24253-33-6 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.102E-01	6.150E+01	19	F300	1 0 0 0 2	

256. $C_4H_5ClO_2$
2-Chlorocrotonic acid
α-Chlor-crotonsaeure
RN: 600-13-5 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-01	2.100E+01	19	F300	1 0 0 0 1	

257. $C_4H_5ClO_2$
3-Chlorocrotonic acid
β-Chlor-crotonsaeure
RN: 6214-28-4 **MP** (°C)**:** 94
MW: 120.54 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-01	2.220E+01	12.5	F300	1 0 0 0 2	
2.481E-01	2.990E+01	19	F300	1 0 0 0 2	

258. $C_4H_5ClO_2$
3-Chloroisocrotonic acid
β-Chlor-isocrotonsaeure
RN: 6625-00-9 **MP** (°C)**:**
MW: 120.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.037E-01	1.250E+01	7	F300	1 0 0 0 2	
1.560E-01	1.880E+01	19	F300	1 0 0 0 2	

259. $C_4H_5ClO_4$
L-Chlorosuccinic acid
L(–)-Chlor-bernsteinsaeure
D-Chlorosuccinic acid
D(+)-Chlor-bernsteinsaeure
RN: 16045-92-4 **MP** (°C)**:**
MW: 152.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E+00	1.800E+02	20	F300	1 0 0 0 1	
1.193E+00	1.820E+02	20	F300	1 0 0 0 2	

260. $C_4H_5F_3O$
Fluroxene
2,2,2-(Trifluoroethoxy)ethene
Redeptin
Fluoromar
RN: 406-90-6 **MP** (°C)**:**
MW: 126.08 **BP** (°C)**:** 42.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.173E-05	4.000E-03	ns	R028	0 0 0 0 0	

261. C_4H_5N
Pyrrole
Azole
Imidole
RN: 109-97-7 **MP** (°C)**:** –23
MW: 67.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.098E-01	4.762E+01	rt	B099	0 2 0 0 0	

262. C_4H_5N

Methacrylonitrile
2-Methyl-2-propenenitrile

RN: 126-98-7 **MP** (°C)**:** –35.8
MW: 67.09 **BP** (°C)**:** 90.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.692E-01	2.477E+01	25	L096	1 2 0 2 2	

263. $C_4H_5NO_2$

Hymexazol
3-Hydroxy-5-methyl isoxazole
5-Methyl-3(2H)-isoxazolone
Tachigaren
Isoxazolol, 5-methyl-

RN: 10004-44-1 **MP** (°C)**:** 86
MW: 99.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-01	8.500E+01	25	M161	1 0 0 0 2	
8.578E-01	8.500E+01	25	N306	1 0 0 0 1	

264. $C_4H_5NO_2$

Succinimide
2,5-Pyrrolidinedione
Butanimide

RN: 123-56-8 **MP** (°C)**:** 126
MW: 99.09 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.174E-01	9.091E+01	0	M043	1 0 0 0 1	
1.392E+00	1.379E+02	10	M043	1 0 0 0 1	
2.082E+00	2.063E+02	20	M043	1 0 0 0 1	
1.978E+00	1.960E+02	21	F300	1 0 0 0 2	
3.273E+00	3.243E+02	30	M043	1 0 0 0 1	
4.577E+00	4.536E+02	40	M043	1 0 0 0 1	
5.887E+00	5.833E+02	60	M043	1 0 0 0 2	
6.868E+00	6.805E+02	80	M043	1 0 0 0 2	
1.413E+00	1.400E+02	ns	D072	0 0 0 0 1	
1.995E+00	1.977E+02	ns	R424	0 0 0 0 0	

265. C_4H_5NS

Allyl isothiocyanate
Allyl mustardiol
Allylsenfoel

RN: 57-06-7 **MP** (°C)**:** –8
MW: 99.16 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.017E-02	2.000E+00	20	F300	1 0 0 0 0	

266. $C_4H_5N_3O$

Cytosine
2-Oxy-4-amino pyrimidine
2(1H)-Pyrimidinone, 4-amino-

RN: 71-30-7 **MP** (°C)**:** 320
MW: 111.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.555E+00	20	C017	2 0 0 1 0	EFG
6.877E-02	7.641E+00	25	D041	1 0 0 0 1	
7.200E-02	8.000E+00	25	F300	1 0 0 0 0	
6.580E-02	7.311E+00	25	H061	0 0 0 0 0	
6.500E-02	7.222E+00	25	R030	0 0 0 0 0	

267. $C_4H_5N_3OS$

6-Amino-2-thiouracil
2-Mercapto-4-amino-6-hydroxypyrimidine
2-Thio-4-amino-6-hydroxypyrimidine
2-Mercapto-6-aminouracil

RN: 1004-40-6 **MP** (°C)**:**
MW: 143.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	2.563E-01	25	G016	1 2 1 2 2	intrinsic

268. $C_4H_5N_3O_2$

5-Aminouracil
5-Amino-uracil

RN: 932-52-5 **MP** (°C)**:** >300
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.934E-03	5.000E-01	20	F300	1 0 0 0 0	
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	
1.259E-01	1.600E+01	100	F300	1 0 0 0 1	

269. $C_4H_5N_3O_2$
6-Aminouracil
2,4(1H,3H)-Pyrimidinedione, 6-amino
4-Amino-2,6-dihydroxypyrimidine
6-Amino-2,4-pyrimidinediol
4-Amino uracil
RN: 873-83-6 **MP** (°C)**:**
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	

270. $C_4H_5N_3O_2$
2-Methyl-4(5)-nitroimidazole
2-Methyl-5-nitroimidazole
Menidazole
RP 8532
L 581490
RN: 696-23-1 **MP** (°C)**:** 257–258
MW: 127.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E-02	3.010E+00	20	D344	0 0 0 0 0	
2.367E-02	3.009E+00	20	D344	0 0 0 0 0	
2.353E-02	2.991E+00	20	D344	0 0 0 0 0	
2.370E-02	3.012E+00	20	D344	0 0 0 0 0	

271. C_4H_6
1,3-Butadiene
Pyrrolylene
RN: 106-99-0 **MP** (°C)**:** –108.9
MW: 54.09 **BP** (°C)**:** –4.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.359E-02	7.350E-01	25	M001	2 1 2 2 2	

272. C_4H_6
1-Butyne
Ethylacetylene
Ethylethyne
RN: 107-00-6 **MP** (°C)**:** –125.7
MW: 54.09 **BP** (°C)**:** 8.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.306E-02	2.870E+00	25	M001	2 1 2 2 2	

273. $C_4H_6BrNO_4$

5-Bromo-5-nitro-1,3-dioxane
Bronidox
Microcide I
Bronidox L
1,3-Dioxane, 5-bromo-5-nitro-
RN: 30007-47-7 **MP** (°C)**:** 49–50
MW: 212.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.706E-02	5.737E+00	25	L013	1 0 2 1 2	

274. $C_4H_6Cl_2O_2S$

3,4-Dichlorotetrahydrothiophene dioxide
3,4-Dichlorotetrahydrothiophene 1,1-dioxide
3,4-Dichlorosulfolane
DAC PRD
3,4-Dichlorothiolane 1,1-dioxide
RN: 3001-57-8 **MP** (°C)**:** 130
MW: 189.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-02	2.195E+00	20	M061	1 0 0 0 1	

275. $C_4H_6N_2O_2$

2,5-Piperazinedione
Diketopiperazine
RN: 106-57-0 **MP** (°C)**:**
MW: 114.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	1.406E+01	20	B032	1 2 2 1 2	
1.253E-01	1.430E+01	20	M075	2 0 1 1 2	
1.475E-01	1.683E+01	25	B032	1 2 2 1 2	
1.754E-01	2.001E+01	29.80	B032	1 2 2 1 2	

276. $C_4H_6N_2S_4Zn$

Zineb
Zinc ethylenebis(dithiocarbamate)
RN: 12122-67-7 **MP** (°C)**:**
MW: 275.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-06	1.000E-03	20	M061	1 0 0 0 0	
3.627E-05	1.000E-02	rt	M161	0 0 0 0 1	

277. $C_4H_6N_4O_3$
Allantoin
Allantoine
RN: 97-59-6 **MP** (°C)**:** 238
MW: 158.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.303E-02	5.223E+00	20	D041	1 0 0 0 2	
4.755E-02	7.519E+00	c	D004	0 0 0 0 0	
2.040E-01	3.226E+01	h	D004	0 0 0 0 0	
2.530E-02	4.000E+00	ns	D072	0 0 0 0 1	

278. $C_4H_6N_4O_3S_2$
Acetazolamide
5-Acetamido-1,3,4-thiadiazole-2-sulfonamide
RN: 59-66-5 **MP** (°C)**:** 258
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.001E-01	15	K024	1 2 1 1 2	
2.249E-03	4.998E-01	20	D041	1 0 0 0 0	
3.200E-03	7.112E-01	25	C415	1 0 0 1 0	
2.216E-03	4.925E-01	25	F415	0 0 0 0 0	Average
4.409E-03	9.799E-01	30	E049	2 0 2 2 2	
5.174E-03	1.150E+00	37	C054	2 0 2 1 2	
2.880E-03	6.400E-01	amb	L434	0 0 0 0 0	
>2.25E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.144E-03	9.210E-01	ns	I304	0 0 0 0 0	
4.500E-04	1.000E-01	ns	K444	0 0 0 0 0	
4.365E-03	9.701E-01	ns	R428	0 0 0 0 0	

279. C_4H_6O
Vinyl ether
1,1′-Oxybisethene
Divinyl ether
RN: 109-93-3 **MP** (°C)**:**
MW: 70.09 **BP** (°C)**:** 28.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.490E-02	5.250E+00	37	R047	0 0 0 0 0	
5.487E-01	3.846E+01	ns	R028	0 0 0 0 0	

280. C_4H_6O
Crotonaldehyde
But-*trans*-enal
RN: 4170-30-3 **MP** (°C)**:** –76.5
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+2.14E+00	+1.50E+02	ns	S460	0 0 0 0 0	

281. C_4H_6O
α-Methylacrolein
α-Methyl-acrolein
RN: 78-85-3 **MP** (°C)**:**
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.089E-01	5.670E+01	20	F300	1 0 0 0 2	
1.236E+00	8.663E+01	ns	S460	0 0 0 0 0	

282. C_4H_6O
trans-Crotonaldehyde
Crotonaldehyd
RN: 123-73-9 **MP** (°C)**:** –77
MW: 70.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.140E+00	1.500E+02	20	F300	1 0 0 0 1	

283. $C_4H_6O_2$
Diacetyl
2,3-Butanedione
RN: 431-03-8 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E+00	2.000E+02	15	F300	1 0 0 0 1	
2.323E+00	2.000E+02	20	D041	1 0 0 0 1	

284. $C_4H_6O_2$
Methyl acrylate
Acrylic acid methyl ester
2-Propenoic acid methyl ester
RN: 96-33-3 **MP** (°C)**:** –76.5
MW: 86.09 **BP** (°C)**:** 70

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.742E-01	4.943E+01	30	L096	1 2 0 2 1	

285. $C_4H_6O_2$
trans-Crotonic acid
trans-Crotonsaeure
RN: 3724-65-0 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.989E-01	8.600E+01	25	F300	1 0 0 0 1	
4.600E+00	3.960E+02	40	F300	1 0 0 0 2	

286. $C_4H_6O_2$
Vinyl acetate
Vinylacetate
RN: 108-05-4 **MP** (°C)**:** –100
MW: 86.09 **BP** (°C)**:** 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.136E-01	2.700E+01	50	L097	1 1 1 1 1	

287. $C_4H_6O_2$
Crotonic acid
2-Butenoic acid
3-Methylacrylic acid
RN: 107-93-7 **MP** (°C)**:** 73
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.882E-01	7.647E+01	20	D041	1 0 0 0 2	

288. $C_4H_6O_2$
α-Butyrolacetone
3-Hydroxybutanoic acid β-lactone
RN: 3068-88-0 **MP** (°C)**:**
MW: 86.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E+00	1.327E+02	18	I313	0 0 0 0 0	

289. $C_4H_6O_2S_4$

bis(Methylxanthogen) disulfide
Dimethylxanthogen disulfide
Methyl dixanthogen

RN: 1468-37-7 **MP** (°C)**:** 22.75
MW: 214.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.465E-02	25	H102	1 2 1 2 2	

290. $C_4H_6O_3$

Acetic anhydride
Essigsaeure-anhydrid

RN: 108-24-7 **MP** (°C)**:** –73
MW: 102.09 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E+00	1.200E+02	20	F300	1 0 0 0 2	

291. $C_4H_6O_4$

Methylmalonic acid
Acide methylmalonique
Methyl-malonsaeure

RN: 516-05-2 **MP** (°C)**:** 129.5
MW: 118.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	3.070E+02	0	F300	1 0 0 0 2	
3.743E+00	4.420E+02	0	M051	1 0 0 0 2	
4.954E+00	5.850E+02	15	M051	1 0 0 0 2	
5.750E+00	6.790E+02	25	M051	1 0 0 0 2	
4.071E+00	4.808E+02	50	F300	1 0 0 0 2	
7.748E+00	9.150E+02	50	M051	1 0 0 0 2	

292. $C_4H_6O_4$

Succinic acid
Bernsteinsaeure

RN: 110-15-6 **MP** (°C)**:** 185
MW: 118.09 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.363E-01	2.790E+01	0	L041	1 0 0 1 2	
2.273E-01	2.684E+01	0	M020	1 0 0 1 1	
2.306E-01	2.724E+01	0	M043	1 0 0 0 1	

(*continued*)

292. $C_4H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.892E-01	3.415E+01	4.99	A339	0 0 0 0 0	
3.569E-01	4.215E+01	10	M043	1 0 0 0 1	
3.616E-01	4.271E+01	9.99	A339	0 0 0 0 0	
3.854E-01	4.551E+01	11.85	L064	2 2 2 1 2	
4.518E-01	5.335E+01	14.99	A339	0 0 0 0 0	
4.102E-01	4.843E+01	15	F055	1 2 2 2 2	
4.149E-01	4.900E+01	15	L041	1 0 0 1 1	
4.149E-01	4.900E+01	15	M051	1 0 0 0 1	
4.912E-01	5.800E+01	17.50	F300	1 0 0 0 1	
4.974E-01	5.874E+01	18	L064	2 2 2 1 2	
5.661E-01	6.685E+01	19.99	A339	0 0 0 0 0	
5.392E-01	6.367E+01	20	D041	1 0 0 0 1	
5.019E-01	5.927E+01	20	F055	1 2 2 2 2	
5.420E-01	6.400E+01	20	F300	1 0 0 0 2	
4.912E-01	5.800E+01	20	L041	1 0 0 1 1	
5.466E-01	6.455E+01	20	M043	1 0 0 0 1	
5.510E-01	6.507E+01	20	M153	1 0 0 0 0	cal. from fitted equation
4.632E-01	5.470E+01	20	M171	1 0 0 0 1	
5.716E-01	6.750E+01	20	W026	1 0 1 1 1	average of 2
6.344E-01	7.492E+01	23.75	L064	2 2 2 1 2	
6.829E-01	8.064E+01	24.99	A339	0 0 0 0 0	
5.930E-01	7.003E+01	25	D061	1 0 0 0 2	
6.032E-01	7.124E+01	25	F055	1 2 2 2 2	
6.849E-01	8.088E+01	25	H430	0 0 0 0 0	
6.518E-01	7.697E+01	25	M020	1 0 0 1 2	
6.634E-01	7.834E+01	25	M153	1 0 0 0 0	cal. from fitted equation
7.402E-01	8.741E+01	28	D050	1 2 1 2 2	
8.003E-01	9.451E+01	29.99	A339	0 0 0 0 0	
8.047E-01	9.502E+01	30	M043	1 0 0 0 2	
8.047E-01	9.502E+01	30	M153	1 0 0 0 0	cal. from fitted equation
8.849E-01	1.045E+02	30	W026	1 0 1 1 2	average of 2
9.508E-01	1.123E+02	34.99	A339	0 0 0 0 0	
8.976E-01	1.060E+02	35	L041	1 0 0 1 2	
9.742E-01	1.150E+02	35	M153	1 0 0 0 0	cal. from fitted equation
1.145E+00	1.353E+02	39.99	A339	0 0 0 0 0	
1.149E+00	1.357E+02	40	B088	1 0 0 0 2	
1.181E+00	1.394E+02	40	M043	1 0 0 0 2	
1.168E+00	1.379E+02	40	M153	1 0 0 0 0	cal. from fitted equation
1.377E+00	1.627E+02	44.99	A339	0 0 0 0 0	
1.600E+00	1.889E+02	49.99	A339	0 0 0 0 0	
1.524E+00	1.800E+02	50	L041	1 0 0 1 2	
1.633E+00	1.929E+02	50	M020	1 0 0 1 2	
1.842E+00	2.175E+02	54.99	A339	0 0 0 0 0	
2.048E+00	2.418E+02	59.99	A339	0 0 0 0 0	
2.232E+00	2.636E+02	60	M043	1 0 0 0 2	
2.398E+00	2.832E+02	64.99	A339	0 0 0 0 0	
2.380E+00	2.810E+02	65	L041	1 0 0 1 2	
3.238E+00	3.824E+02	75	F300	1 0 0 0 2	
3.191E+00	3.768E+02	75	M020	1 0 0 1 2	

(*continued*)

292. $C_4H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E+00	4.145E+02	80	M043	1 0 0 0 2	
8.515E-01	1.006E+02	84.30	B118	1 0 0 0 2	unit assumed
4.636E+00	5.475E+02	100	D041	1 0 0 0 2	
4.738E+00	5.595E+02	100	M043	1 0 0 0 2	
6.821E-01	8.054E+01	rt	H431	0 0 0 0 0	

293. $C_4H_6O_4$

Methyl oxalate
Oxalic acid ethyl ester
Oxalsaeure-monoaethyl ester

RN: 553-90-2 **MP** (°C)**:** 54.0
MW: 118.09 **BP** (°C)**:** 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-01	3.549E+01	.1	K079	1 0 0 0 2	
6.900E-01	8.148E+01	11.1	K079	1 0 0 0 2	
1.029E+00	1.216E+02	19.5	K079	1 0 0 0 2	
5.106E-01	6.030E+01	25	F300	1 0 0 0 2	
1.489E+00	1.758E+02	27.1	K079	1 0 0 0 2	
1.867E+00	2.204E+02	31.9	K079	1 0 0 0 2	
2.978E+00	3.516E+02	44.4	K079	1 0 0 0 2	
3.372E+00	3.982E+02	49.2	K079	1 0 0 0 2	
3.589E+00	4.238E+02	51.0	K079	1 0 0 0 2	
3.839E+00	4.533E+02	53.0	K079	1 0 0 0 2	
4.783E+00	5.649E+02	75.0	K079	1 0 0 0 2	
4.939E+00	5.832E+02	79.3	K079	1 0 0 0 2	
5.678E+00	6.705E+02	96.1	K079	1 0 0 0 2	
4.929E-01	5.820E+01	rt	D021	0 0 1 1 2	

294. $C_4H_6O_5$

D-Malic acid
D(–)-Aepfelsaeure

RN: 636-61-3 **MP** (°C)**:** 100
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.397E+00	4.555E+02	4.99	A339	0 0 0 0 0	
3.542E+00	4.749E+02	9.99	A339	0 0 0 0 0	
3.695E+00	4.954E+02	14.99	A339	0 0 0 0 0	
3.878E+00	5.200E+02	19.99	A339	0 0 0 0 0	
4.030E+00	5.403E+02	24.99	A339	0 0 0 0 0	
4.146E+00	5.560E+02	29.99	A339	0 0 0 0 0	
4.282E+00	5.742E+02	34.99	A339	0 0 0 0 0	
4.441E+00	5.955E+02	39.99	A339	0 0 0 0 0	
4.544E+00	6.094E+02	44.99	A339	0 0 0 0 0	

(*continued*)

294. $C_4H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E+00	6.328E+02	49.99	A339	0 0 0 0 0	
4.840E+00	6.490E+02	54.99	A339	0 0 0 0 0	
4.976E+00	6.672E+02	59.99	A339	0 0 0 0 0	
5.119E+00	6.865E+02	64.99	A339	0 0 0 0 0	

295. $C_4H_6O_5$

Diglycolic acid
Di-glykolsaeure

RN: 110-99-6 **MP** (°C)**:** 148
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E+00	2.140E+02	5.09	A340	0 0 0 0 0	
1.932E+00	2.590E+02	10.99	A340	0 0 0 0 0	
2.522E+00	3.382E+02	15.59	A340	0 0 0 0 0	
2.668E+00	3.577E+02	20.59	A340	0 0 0 0 0	
2.834E+00	3.801E+02	23.49	A340	0 0 0 0 0	
3.252E+00	4.361E+02	28.09	A340	0 0 0 0 0	
3.645E+00	4.887E+02	37.49	A340	0 0 0 0 0	
3.794E+00	5.087E+02	39.99	A340	0 0 0 0 0	
4.061E+00	5.445E+02	47.99	A340	0 0 0 0 0	
4.135E+00	5.545E+02	49.99	A340	0 0 0 0 0	
4.353E+00	5.837E+02	54.49	A340	0 0 0 0 0	
4.508E+00	6.044E+02	59.49	A340	0 0 0 0 0	
4.631E+00	6.209E+02	64.99	A340	0 0 0 0 0	
4.776E+00	6.404E+02	69.99	A340	0 0 0 0 0	
4.877E+00	6.540E+02	74.99	A340	0 0 0 0 0	
4.969E+00	6.663E+02	79.89	A340	0 0 0 0 0	
5.067E+00	6.794E+02	83.99	A340	0 0 0 0 0	
5.125E+00	6.872E+02	88.19	A340	0 0 0 0 0	

296. $C_4H_6O_5$

DL-Malic acid
Malic acid

RN: 6915-15-7 **MP** (°C)**:** 131.5
MW: 134.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.512E+00	4.709E+02	0	M043	1 0 0 0 1	
3.820E+00	5.122E+02	10	M043	1 0 0 0 2	
4.158E+00	5.575E+02	20	M043	1 0 0 0 2	
4.414E+00	5.918E+02	25	H430	0 0 0 0 0	
4.401E+00	5.902E+02	26	D041	1 0 0 0 2	
4.415E+00	5.920E+02	26	F300	1 0 0 0 2	

(*continued*)

296. $C_4H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.605E+00	7.516E+02	30	D062	1 0 1 1 0	data given in normality
4.475E+00	6.000E+02	30	M043	1 0 0 0 2	
4.794E+00	6.429E+02	40	M043	1 0 0 0 2	
5.442E+00	7.297E+02	60	M043	1 0 0 0 2	
5.998E+00	8.043E+02	79	D041	1 0 0 0 2	
6.033E+00	8.089E+02	79	F300	1 0 0 0 2	
6.126E+00	8.214E+02	80	M043	1 0 0 0 2	

297. $C_4H_6O_6$

meso-Tartaric acid
meso-Weinsaeure

RN: 147-73-9 **MP** (°C)**:** 147
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	3.360E+02	0	F300	1 0 0 0 2	
3.702E+00	5.556E+02	15	D041	1 0 0 0 2	
3.731E+00	5.600E+02	15	F300	1 0 0 0 1	
3.731E+00	5.600E+02	20	F300	1 0 0 0 1	

298. $C_4H_6O_6$

D-(–)-Tartaric acid
D-(–)-Dihydroxysuccinic acid

RN: 147-71-7 **MP** (°C)**:** 173
MW: 150.09 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.564E+00	5.349E+02	0	M043	1 0 0 0 2	
3.348E+00	5.024E+02	4.99	A339	0 0 0 0 0	
2.350E+00	3.528E+02	10	D020	1 2 1 1 2	
3.715E+00	5.575E+02	10	M043	1 0 0 0 2	
3.431E+00	5.149E+02	9.99	A339	0 0 0 0 0	
3.499E+00	5.251E+02	14.99	A339	0 0 0 0 0	
3.553E+00	5.332E+02	19.99	A339	0 0 0 0 0	
3.875E+00	5.816E+02	20	M043	1 0 0 0 2	
3.629E+00	5.447E+02	24.99	A339	0 0 0 0 0	
2.459E+00	3.691E+02	25	D020	1 2 1 1 2	
3.973E+00	5.963E+02	25	F017	1 0 0 0 2	
3.706E+00	5.562E+02	29.99	A339	0 0 0 0 0	
4.060E+00	6.094E+02	30	M043	1 0 0 0 2	
3.791E+00	5.690E+02	34.99	A339	0 0 0 0 0	
3.846E+00	5.773E+02	39.99	A339	0 0 0 0 0	
4.249E+00	6.377E+02	40	M043	1 0 0 0 2	
3.926E+00	5.892E+02	44.99	A339	0 0 0 0 0	

(*continued*)

298. $C_4H_6O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E+00	6.036E+02	49.99	A339	0 0 0 0 0	
4.104E+00	6.160E+02	54.99	A339	0 0 0 0 0	
4.157E+00	6.238E+02	59.99	A339	0 0 0 0 0	
4.581E+00	6.875E+02	60	M043	1 0 0 0 2	
4.232E+00	6.352E+02	64.99	A339	0 0 0 0 0	
4.876E+00	7.319E+02	80	M043	1 0 0 0 2	
5.159E+00	7.743E+02	100	M043	1 0 0 0 2	

299. $C_4H_6O_6$

L-Tartaric acid
L(+)-Weinsaeure
L(+)-Tartaric acid

RN: 87-69-4 **MP** (°C)**:** 169
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.565E+00	5.350E+02	0	F300	1 0 0 0 2	
3.564E+00	5.349E+02	0	F302	1 0 0 0 2	
3.634E+00	5.455E+02	5	F302	1 0 0 0 2	
3.702E+00	5.556E+02	10	F302	1 0 0 0 2	
3.791E+00	5.690E+02	15	F302	1 0 0 0 2	
3.878E+00	5.820E+02	20	F300	1 0 0 0 2	
3.875E+00	5.816E+02	20	F302	1 0 0 0 2	
3.965E+00	5.951E+02	25	F302	1 0 0 0 2	
4.060E+00	6.094E+02	30	F302	1 0 0 0 2	
4.158E+00	6.241E+02	35	F302	1 0 0 0 2	
4.249E+00	6.377E+02	40	F302	1 0 0 0 2	
4.325E+00	6.491E+02	45	F302	1 0 0 0 2	
4.397E+00	6.600E+02	50	F300	1 0 0 0 1	
4.404E+00	6.610E+02	50	F302	1 0 0 0 2	
4.485E+00	6.732E+02	55	F302	1 0 0 0 2	
4.568E+00	6.855E+02	60	F302	1 0 0 0 2	
4.644E+00	6.970E+02	65	F302	1 0 0 0 2	
4.726E+00	7.093E+02	70	F302	1 0 0 0 2	
4.802E+00	7.207E+02	75	F302	1 0 0 0 2	
4.876E+00	7.319E+02	80	F302	1 0 0 0 2	
4.954E+00	7.436E+02	85	F302	1 0 0 0 2	
5.026E+00	7.543E+02	90	F302	1 0 0 0 2	
5.095E+00	7.647E+02	95	F302	1 0 0 0 2	
5.157E+00	7.740E+02	100	F300	1 0 0 0 2	
5.159E+00	7.743E+02	100	F302	1 0 0 0 2	

300. $C_4H_6O_6$

DL-Tartaric acid
DL-Weinsaeure
Tartaric acid (racemic)

RN: 133-37-9 **MP** (°C)**:** 206
MW: 150.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.279E+00	3.421E+02	0	D039	2 2 1 2 0	EFG
5.630E-01	8.450E+01	0	D041	1 0 0 0 2	
5.084E-01	7.630E+01	0	F300	1 0 0 0 2	
5.049E-01	7.579E+01	0	M043	1 0 0 0 1	
2.333E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
7.298E-01	1.095E+02	10	M043	1 0 0 0 2	
2.350E+00	3.528E+02	20	D039	2 2 1 2 0	EFG
1.138E+00	1.708E+02	20	D041	1 0 0 0 2	
1.139E+00	1.710E+02	20	F300	1 0 0 0 2	
1.016E+00	1.525E+02	20	M043	1 0 0 0 2	
2.459E+00	3.690E+02	25	D039	2 2 1 2 2	EFG
1.179E+00	1.770E+02	25	F017	1 0 0 0 2	
1.026E+01	1.540E+03	25	K040	1 0 2 1 2	
2.483E+00	3.726E+02	30	D039	2 2 1 2 0	EFG
1.341E+00	2.013E+02	30	M043	1 0 0 0 2	
2.563E+00	3.846E+02	40	D039	2 2 1 2 0	EFG
1.799E+00	2.701E+02	40	M043	1 0 0 0 2	
2.612E+00	3.921E+02	50	D039	2 2 1 2 0	EFG
2.687E+00	4.033E+02	60	D039	2 2 1 2 0	EFG
2.612E+00	3.921E+02	60	M043	1 0 0 0 2	
2.750E+00	4.128E+02	70	D039	2 2 1 2 0	EFG
2.811E+00	4.220E+02	80	D039	2 2 1 2 0	EFG
3.299E+00	4.952E+02	80	M043	1 0 0 0 2	
2.860E+00	4.292E+02	90	D039	2 2 1 2 0	EFG
2.920E+00	4.382E+02	100	D039	2 2 1 2 0	EFG
4.324E+00	6.490E+02	100	D041	1 0 0 0 2	
4.331E+00	6.500E+02	100	F300	1 0 0 0 1	
3.863E+00	5.798E+02	100	M043	1 0 0 0 2	

301. C_4H_7Br

4-Bromo-1-butene
1-Bromo-3-butene
Homoallyl bromide
4-Bromobutene-1
3-Butenyl bromide

RN: 5162-44-7 **MP** (°C)**:**
MW: 135.01 **BP** (°C)**:** 98.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.660E-03	7.642E-01	25	M342	1 0 1 1 2	

302. $C_4H_7BrN_2O_2$

Propanamide, *N*-(aminocarbonyl)-2-bromo-
(2-Bromopropionyl)urea
α-Bromopropionylurea

RN: 14299-55-9 **MP** (°C)**:**
MW: 195.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.581E-01	5.033E+01	ns	F056	0 2 2 2 1	

303. $C_4H_7BrO_2$

α-Bromobutyric acid
DL-2-Bromobutyric acid
DL-Brombuttersaeure

RN: 80-58-0 **MP** (°C)**:** –4
MW: 167.01 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.191E-01	7.000E+01	ns	F300	1 0 0 0 0	

304. C_4H_7Cl

1-Chloro-2-butene
1-Chloro-2-methylpropene-2
α-Methylallyl chloride

RN: 591-97-9 **MP** (°C)**:**
MW: 90.55 **BP** (°C)**:** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-02	9.990E-01	ns	M061	0 0 0 0 0	

305. $C_4H_7Cl_2O_4P$

Dichlorvos
O,O-Dimethyl *O*-2-dichlorovinyl phosphate

RN: 62-73-7 **MP** (°C)**:**
MW: 220.98 **BP** (°C)**:** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-02	9.901E+00	ns	M061	0 0 0 0 0	
4.525E-02	1.000E+01	rt	M161	0 0 0 0 1	

306. $C_4H_7Cl_3O$

1,1,1-Trichloro-*tert*-butanol
Acetonchloroform
Chloreton

RN: 57-15-8 **MP** (°C)**:** 98
MW: 177.46 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.508E-02	8.000E+00	20	F300	1 0 0 0 0	
4.467E-02	7.927E+00	ns	R424	0 0 0 0 0	
4.467E-02	7.927E+00	ns	R427	0 0 0 0 0	

307. C_4H_7N

n-Butyroniitrile
γ-Butyronitrile
Propyl cyanide
1-Cyanopropane
n-Butyronitrile

RN: 109-74-0 **MP** (°C)**:** –112
MW: 69.11 **BP** (°C)**:** 115–117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.446E-02	3.764E+00	25	B004	0 0 0 0 0	

308. $C_4H_7NO_2S$

4-Thiazolidinecarboxylic acid
Thiazolidine-4-carboxylic acid
γ-Thiaproline
4-Carboxythiazolidine
Detoxepa
Thiaproline

RN: 444-27-9 **MP** (°C)**:** 196–201
MW: 133.17 **BP** (°C)**:** 350.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.930E+01	21	B414	1 0 0 1 1	

309. $C_4H_7NO_3$

N-Acetyl glycine
Aceturic acid
Glycin-*N*-acetat
Glycine-*N*-acetate

RN: 543-24-8 **MP** (°C)**:** 206
MW: 117.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.246E-01	2.630E+01	15	F300	1 0 0 0 2	

310. $C_4H_7NO_4$

Butanoic acid, 4-amino-2-hydroxy-4-oxo-
D-β-Malaminsaeure
r-β-Malaminsaeure

RN: 82310-91-6 **MP** (°C)**:** 149
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.903E-01	3.865E+01	18	L039	1 0 0 0 2	
5.255E-01	6.994E+01	18	L039	1 0 0 0 2	

311. $C_4H_7NO_4$

DL-Aspartic acid
DL-2-Aminobutanedioic acid

RN: 617-45-8 **MP** (°C)**:**
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.367E-02	3.151E+00	0	D018	2 2 2 1 2	
2.420E-02	3.221E+00	4.99	A405	2 0 1 1 2	
3.140E-02	4.179E+00	9.99	A405	2 0 1 1 2	
3.910E-02	5.204E+00	14.99	A405	2 0 1 1 2	
4.850E-02	6.456E+00	19.99	A405	2 0 1 1 2	
5.900E-02	7.853E+00	24.99	A405	2 0 1 1 2	
6.081E-02	8.094E+00	25	D018	2 2 2 1 2	
6.110E-02	8.133E+00	25	D041	1 0 0 0 1	
7.260E-02	9.663E+00	29.99	A405	2 0 1 1 2	
8.770E-02	1.167E+01	33.99	A405	2 0 1 1 2	
8.950E-02	1.191E+01	34.99	A405	2 0 1 1 2	
1.069E-01	1.423E+01	38.99	A405	2 0 1 1 2	
1.109E-01	1.476E+01	39.99	A405	2 0 1 1 2	
1.293E-01	1.721E+01	44.99	A405	2 0 1 1 2	
1.561E-01	2.078E+01	49.49	A405	2 0 1 1 2	
1.544E-01	2.055E+01	50	D018	2 2 2 1 2	
1.812E-01	2.412E+01	54.99	A405	2 0 1 1 2	
2.170E-01	2.888E+01	58.99	A405	2 0 1 1 2	

(*continued*)

311. $C_4H_7NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.543E-01	3.385E+01	61.99	A405	2 0 1 1 2	
3.101E-01	4.128E+01	65.99	A405	2 0 1 1 2	
3.284E-01	4.371E+01	68.99	A405	2 0 1 1 2	
3.646E-01	4.853E+01	70.99	A405	2 0 1 1 2	
3.437E-01	4.575E+01	75	D018	2 2 2 1 2	
3.434E-01	4.571E+01	75	D041	1 0 0 0 2	

312. $C_4H_7NO_4$

Iminodiacetic acid
Imino-diessigsaeure

RN: 142-73-4 **MP** (°C)**:** 247.5
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.781E-01	2.370E+01	5	F300	1 0 0 0 2	

313. $C_4H_7NO_4$

L-Aspartic acid
Aspartic acid
L(+)-Asparaginsaeure
L-(+)-Asparaginic acid
L-(+)-Aspartic acid

RN: 56-84-8 **MP** (°C)**:** 270.5
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-02	2.230E+00	0	D018	2 2 2 1 2	
1.780E-02	2.369E+00	4.99	A405	2 0 1 1 2	
2.170E-02	2.888E+00	9.99	A405	2 0 1 1 2	
2.570E-02	3.421E+00	14.99	A405	2 0 1 1 2	
3.160E-02	4.206E+00	19.99	A405	2 0 1 1 2	
3.170E-02	4.220E+00	20	B032	1 2 2 1 2	
3.750E-02	4.991E+00	24.99	A405	2 0 1 1 2	
3.770E-02	5.018E+00	25	B032	1 2 2 1 2	
4.030E-02	5.364E+00	25	D018	2 2 2 1 2	
3.738E-02	4.975E+00	25	D041	1 0 0 0 0	
3.805E-02	5.064E+00	25	G315	0 0 0 0 0	
3.719E-02	4.950E+00	25	J303	0 0 0 0 0	
3.644E-02	4.850E+00	27	D036	0 0 0 0 0	
4.469E-02	5.948E+00	29.80	B032	1 2 2 1 2	
4.550E-02	6.056E+00	29.99	A405	2 0 1 1 2	
5.320E-02	7.081E+00	33.99	A405	2 0 1 1 2	
6.520E-02	8.678E+00	39.99	A405	2 0 1 1 2	
6.348E-02	8.450E+00	40	J303	0 0 0 0 0	

(*continued*)

313. $C_4H_7NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.610E-02	1.013E+01	44.99	A405	2 0 1 1 2	
9.304E-02	1.238E+01	50	D018	2 2 2 1 2	
9.110E-02	1.213E+01	50.99	A405	2 0 1 1 2	
1.013E-01	1.348E+01	54.99	A405	2 0 1 1 2	
1.216E-01	1.619E+01	59.99	A405	2 0 1 1 2	
1.232E-01	1.640E+01	60	J303	0 0 0 0 0	
1.316E-01	1.752E+01	62.99	A405	2 0 1 1 2	
1.440E-01	1.917E+01	64.99	A405	2 0 1 1 2	
1.498E-01	1.994E+01	66.99	A405	2 0 1 1 2	
1.725E-01	2.296E+01	69.99	A405	2 0 1 1 2	
1.985E-01	2.642E+01	75	D018	2 2 2 1 2	
2.100E-01	2.795E+01	75	D041	1 0 0 0 2	
2.885E-01	3.840E+01	99	M160	2 1 1 1 0	
3.750E-02	4.991E+00	ns	M025	0 2 0 1 2	
3.738E-02	4.975E+00	rt	H431	0 0 0 0 0	

314. $C_4H_7NO_4$

L-β-Malamidic acid
L-β-Malaminsaeure

RN: 57229-74-0 **MP** (°C)**:** 149
MW: 133.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.242E-01	6.977E+01	18	L039	1 0 0 0 2	

315. $C_4H_7N_2O_4$

Glycine dipeptide

RN: **MP** (°C)**:**
MW: 147.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E+00	2.086E+02	20	B032	1 2 2 1 2	
1.534E+00	2.257E+02	25	B032	1 2 2 1 2	
1.540E+00	2.266E+02	25.1	N024	0 0 0 0 0	
1.546E+00	2.275E+02	25.1	N026	0 0 0 0 0	
1.647E+00	2.423E+02	29.80	B032	1 2 2 1 2	

316. $C_4H_7N_3O$
Creatinine
Kreatinin
RN: 60-27-5 **MP** (°C)**:** 220.5
MW: 113.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.075E-01	8.004E+01	16	D041	1 0 0 0 1	
7.081E-01	8.010E+01	16	F300	1 0 0 0 2	

317. C_4H_8
1-Butene
α-Butene
Ethylethylene
α-Butylene
1-Butylene
Butene-1
RN: 106-98-9 **MP** (°C)**:** –185
MW: 56.11 **BP** (°C)**:** –6.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.957E-03	2.220E-01	25	M001	2 1 2 2 2	
1.210E-02	6.791E-01	38	B123	1 2 1 1 2	
1.582E-02	8.876E-01	71	B123	1 2 1 1 2	
2.746E-02	1.541E+00	104	B123	1 2 1 1 2	
3.526E-02	1.979E+00	138	B123	1 2 1 1 2	
3.858E-02	2.165E+00	144.00	B123	1 2 1 1 2	

318. C_4H_8
Isobutylene
2-Methylpropene
RN: 115-11-7 **MP** (°C)**:** –140.3
MW: 56.11 **BP** (°C)**:** –6.90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-03	2.630E-01	25	M001	2 1 2 2 2	

319. $C_4H_8Cl_2$

2,3-Dichlorobutane
Butane, 2,3-dichloro-
RN: 7581-97-7 **MP** (°C)**:** –80
MW: 127.01 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-02	1.817E+00	0	L103	1 0 0 0 2	unit assumed
4.422E-03	5.617E-01	20	L103	1 0 0 0 2	unit assumed
1.464E-03	1.860E-01	30	L103	1 0 0 0 2	unit assumed
1.755E-03	2.230E-01	40	L103	1 0 0 0 2	unit assumed

320. $C_4H_8Cl_2O$

sym-Dichloroethyl ether
2,2′-Dichlorodiethylether
RN: 111-44-4 **MP** (°C)**:** –50
MW: 143.01 **BP** (°C)**:** 66

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.060E-02	1.010E+01	20	D052	1 1 0 0 0	
7.403E-02	1.059E+01	20	M062	1 0 0 0 2	

321. $C_4H_8Cl_2OS$

β,β′-Dichlorodiethylsulfoxide
β,β′-Dichlor-diaethylsulfoxid
RN: 5819-08-9 **MP** (°C)**:**
MW: 175.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.854E-02	1.200E+01	20	F300	1 0 0 0 1	

322. $C_4H_8Cl_2O_2S$

β,β′-Dichlorodiethylsulfone
β,β′-Dichlor-diaethylsulfon
RN: 471-03-4 **MP** (°C)**:**
MW: 191.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.140E-02	6.000E+00	20	F300	1 0 0 0 0	
1.256E-01	2.400E+01	100	F300	1 0 0 0 1	

323. $C_4H_8Cl_2S$

Mustard gas
Sulfure β′-ethyl dichlore
β,β′-Dichlor-diaethylsulfid
RN: 505-60-2 **MP** (°C)**:**
MW: 159.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.337E-03	6.900E-01	25	F300	1 0 0 0 1	
3.017E-03	4.800E-01	c	B079	0 0 1 1 1	

324. $C_4H_8Cl_3O_4P$

Trichlorfon
O,O-Dimethyl (1-hydroxy-2,2,2-trichloroethyl)phosphonate
RN: 52-68-6 **MP** (°C)**:** 83.5
MW: 257.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.982E-01	1.540E+02	25	M161	1 0 0 0 2	
4.255E-01	1.095E+02	ns	M061	0 0 0 0 2	

325. $C_4H_8N_2O_2$

Dimethylglyoxime
Dimethylglyoxim
RN: 95-45-4 **MP** (°C)**:** 240.5
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.167E-03	6.000E-01	20	F300	1 0 0 0 0	
3.100E-02	3.600E+00	80	F300	1 0 0 0 1	
5.081E-02	5.900E+00	100	F300	1 0 0 0 1	

326. $C_4H_8N_2O_2$

Succinamide
Bersteinsaeure-diamid
RN: 110-14-5 **MP** (°C)**:** 260
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.858E-02	4.480E+00	15	D041	1 0 0 0 1	
2.842E-02	3.300E+00	15	F300	1 0 0 0 1	
8.534E-01	9.910E+01	100	D041	1 0 0 0 2	
3.445E-04	4.000E-02	c	L055	0 0 0 0 2	
9.463E-03	1.099E+00	h	L055	0 0 0 0 1	
2.818E-02	3.273E+00	ns	R424	0 0 0 0 0	

327. $C_4H_8N_2O_3$
β-Alanine hydantoic acid
β-Uramidopropionic acid
Glycine, *N*-(aminocarbonyl)-*N*-methyl-
RN: 30565-25-4 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	2.087E+01	25	M024	1 2 0 1 2	

328. $C_4H_8N_2O_3$
N-Nitroso-*N*-methylurethane
N-Nitroso-*N*-methyl-urethan
RN: 615-53-2 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	3.699E+01	24	M031	1 1 1 1 1	

329. $C_4H_8N_2O_3$
N-Glycylglycine
Diglycine
RN: 556-50-3 **MP** (°C)**:** 215
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E+00	1.656E+02	21	F300	1 0 0 0 2	
1.740E+00	2.299E+02	24.99	B441	0 0 0 0 0	
1.399E+00	1.848E+02	25	G092	2 1 1 1 1	
1.399E+00	1.848E+02	25	G315	0 0 0 0 0	
1.430E+00	1.890E+02	25.1	N027	1 2 2 2 2	
1.512E+00	1.998E+02	ns	M025	0 2 0 1 2	

330. $C_4H_8N_2O_3$
α-Alanine hydantoic acid
Methylhydantoic acid
RN: 77340-50-2 **MP** (°C)**:**
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-01	2.550E+01	25	M024	1 2 0 1 2	
1.930E-01	2.550E+01	ns	M025	0 2 0 1 2	

331. $C_4H_8N_2O_3$

Asparagine
L-Asparagine
L-Asparagin

RN: 70-47-3 **MP** (°C)**:** 235
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.509E-02	8.600E+00	0	F300	1 0 0 0 1	
2.180E-01	2.880E+01	15	D349	2 1 1 2 2	
1.759E-01	2.324E+01	20	B032	1 2 2 1 2	
2.210E-01	2.920E+01	20	D349	2 1 1 2 2	
1.589E-01	2.100E+01	20	F300	1 0 0 0 2	
8.477E-02	1.120E+01	21.5	P045	0 0 2 1 2	
2.226E-01	2.941E+01	25	B032	1 2 2 1 2	
2.260E-01	2.986E+01	25	D349	2 1 1 2 2	
1.709E-01	2.258E+01	25	G315	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N024	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N025	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N026	0 0 0 0 0	
1.853E-01	2.449E+01	25.1	N027	1 1 2 2 2	
1.918E-01	2.534E+01	27	D036	0 0 0 0 0	
2.233E-01	2.950E+01	27	D036	0 0 0 0 0	
2.777E-01	3.669E+01	29.80	B032	1 2 2 1 2	
2.604E+00	3.440E+02	98	F300	1 0 0 0 2	
1.817E-01	2.400E+01	ns	D072	0 0 0 0 1	
1.860E-01	2.457E+01	ns	M025	0 2 0 1 2	
1.774E-01	2.344E+01	rt	D021	0 0 1 1 2	

332. $C_4H_8N_2O_3.H_2O$

L-Asparagine monohydrate
Asparagine, monohydrate, L-

RN: 5794-13-8 **MP** (°C)**:** 234
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-01	2.902E+01	25	D041	1 0 0 0 2	
1.858E-01	2.790E+01	25	O316	1 0 1 2 2	
1.853E-01	2.781E+01	25	O316	1 0 1 2 2	
1.293E+00	1.941E+02	75	D041	1 0 0 0 2	

333. $C_4H_8N_4O_2$

N,N′-Dinitrosopiperazine
Dinitrosopiperazine

RN: 140-79-4 **MP** (°C)**:**
MW: 144.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	5.765E+00	24	D083	2 0 0 0 1	

334. C_4H_8O

2-Butyraldehyde
Butyraldehyde
Butyraldehyd
n-Butanal

RN: 123-72-8 **MP** (°C)**:** –96
MW: 72.11 **BP** (°C)**:** 75

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-01	3.568E+01	20	D041	1 0 0 0 1	
4.993E-01	3.600E+01	20	F300	1 0 0 0 1	
9.694E-01	6.990E+01	25	A049	1 0 0 0 2	
9.194E-01	6.629E+01	25	B060	2 0 1 1 1	
5.077E-01	3.661E+01	38	J020	2 2 2 1 1	

335. C_4H_8O

Ethyl vinyl ether
Aethyl-vinyl-aether

RN: 109-92-2 **MP** (°C)**:** –115.0
MW: 72.11 **BP** (°C)**:** 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	1.002E+01	37	E028	1 1 2 2 2	

336. C_4H_8O

Isobutyraldehyde
2-Methyl propanal

RN: 78-84-2 **MP** (°C)**:** –66
MW: 72.11 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	8.413E+01	20	M146	1 2 2 2 2	
1.234E+00	8.900E+01	25	A049	1 0 0 0 0	

337. C_4H_8O

Methyl ethyl ketone
Butanon-(2)

RN: 78-93-3 **MP** (°C)**:** –87
MW: 72.11 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
5.780E+00	4.168E+02	4	C423	0 0 0 0 0	
4.338E+00	3.128E+02	10	C423	0 0 0 0 0	
1.015E+00	7.322E+01	20	A075	1 0 0 0 1	

(*continued*)

337. C_4H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E+00	2.038E+02	20	D052	1 1 0 0 2	
2.922E+00	2.107E+02	20	E019	1 0 1 1 2	
2.399E+00	1.730E+02	20	F300	1 0 0 0 2	
2.977E+00	2.146E+02	20	G030	1 2 0 0 2	
5.020E+00	3.620E+02	20	P040	0 0 0 0 0	
2.931E+00	2.114E+02	25	A094	1 0 0 0 2	
3.302E+00	2.381E+02	25	A356	0 0 0 0 0	
2.931E+00	2.114E+02	25	B060	2 0 1 1 1	
3.732E+00	2.691E+02	25	C435	0 0 0 0 0	
3.130E+00	2.257E+02	25	F044	1 0 0 0 2	
2.824E+00	2.036E+02	25	G030	1 2 0 0 2	
2.657E+00	1.916E+02	25	J005	1 0 2 1 2	
6.112E+00	4.407E+02	25	K105	2 0 0 0 2	
2.912E+00	2.100E+02	25	M136	2 0 0 0 2	
2.912E+00	2.100E+02	25	M139	2 0 0 0 2	
2.720E+00	1.961E+02	25	N309	1 0 0 0 2	
2.756E+00	1.987E+02	25	O028	2 2 2 2 2	
2.556E+00	1.843E+02	25	P055	1 0 0 0 1	
2.774E+00	2.000E+02	25	R320	1 0 1 1 2	
2.690E+00	1.940E+02	30	G030	1 2 0 0 2	
1.703E+00	1.228E+02	30	R319	2 2 2 1 2	
2.900E+00	2.091E+02	35	A356	0 0 0 0 0	
2.969E+00	2.141E+02	35	C309	2 2 2 2 1	
2.538E+00	1.830E+02	38	J020	2 0 2 1 2	
7.726E-01	5.571E+01	40	A075	1 0 0 0 1	
2.723E+00	1.964E+02	45	A356	0 0 0 0 0	
2.615E+00	1.885E+02	45	C309	2 2 2 2 1	
6.257E+00	4.512E+02	45	K105	2 0 0 0 2	
6.855E-01	4.943E+01	60	A075	1 0 0 0 1	
6.319E+00	4.556E+02	60	K105	2 0 0 0 2	
6.352E-01	4.580E+01	70	A075	1 0 0 0 1	
3.453E+00	2.490E+02	70	P040	0 0 0 0 0	
2.219E+00	1.600E+02	90	F300	1 0 0 0 1	
3.627E+00	2.615E+02	100	P040	0 0 0 0 0	
6.844E+00	4.935E+02	140	P040	0 0 0 0 0	
3.334E+00	2.404E+02	ns	C309	2 2 2 2 1	
+1.89E+00	+1.36E+02	ns	S460	0 0 0 0 0	

338. C_4H_8O

Tetrahydrofuran
1,4-Epoxybutane
Butylene oxide

RN: 109-99-9 **MP** (°C)**:** –108.0
MW: 72.11 **BP** (°C)**:** 66.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E+00	3.243E+02	72.2	M347	2 2 2 1 2	
4.504E+00	3.248E+02	72.25	M347	2 2 2 1 2	

(*continued*)

338. C_4H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E+00	3.271E+02	72.3	M347	2 2 2 1 2	
4.251E+00	3.065E+02	73.4	M347	2 2 2 1 2	
4.019E+00	2.898E+02	75.4	M347	2 2 2 1 2	
3.678E+00	2.652E+02	78.6	M347	2 2 2 1 2	
3.595E+00	2.593E+02	78.9	M347	2 2 2 1 2	
3.378E+00	2.436E+02	83.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	87.9	M347	2 2 2 1 2	
3.217E+00	2.320E+02	89.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	92.9	M347	2 2 2 1 2	
3.042E+00	2.194E+02	102.5	M347	2 2 2 1 2	
3.042E+00	2.194E+02	110.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	119.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	127.8	M347	2 2 2 1 2	
3.595E+00	2.593E+02	132.9	M347	2 2 2 1 2	
3.998E+00	2.883E+02	136.1	M347	2 2 2 1 2	
4.067E+00	2.933E+02	136.5	M347	2 2 2 1 2	
4.617E+00	3.329E+02	137.1	M347	2 2 2 1 2	
6.934E+00	5.000E+02	rt	B066	0 2 0 0 2	

339. $C_4H_8O_2$

Ethyl acetate
Athylacetat
Essigsaeureaethyl ester

RN: 141-78-6 **MP** (°C)**:** –83
MW: 88.11 **BP** (°C)**:** 77

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.941E-01	8.759E+01	0	B108	1 2 0 1 1	
1.097E+00	9.666E+01	0	B108	1 2 0 1 2	
1.919E+00	1.691E+02	0	C423	0 0 0 0 0	
1.069E+00	9.420E+01	0	G062	1 2 2 2 2	
1.032E+00	9.091E+01	0	M088	2 0 0 0 1	
1.144E+00	1.008E+02	0	M111	1 0 1 1 2	
1.054E+00	9.290E+01	4	C423	0 0 0 0 0	
8.297E-01	7.310E+01	10	C423	0 0 0 0 0	
9.333E-01	8.223E+01	10	G062	1 2 2 2 2	
1.001E+00	8.817E+01	10	M111	1 0 1 1 2	
9.944E-01	8.762E+01	10.0	K079	1 0 0 0 2	
8.698E-01	7.664E+01	15	M088	2 0 0 0 1	
9.419E-01	8.299E+01	15	M111	1 0 1 1 2	
8.329E-01	7.339E+01	17.0	G101	1 2 1 1 2	
8.718E-01	7.681E+01	20	A016	1 2 1 1 2	
8.212E-01	7.236E+01	20	B108	1 2 0 1 1	
8.795E-01	7.749E+01	20	B108	1 2 0 1 2	
7.346E-01	6.472E+01	20	D052	1 1 0 0 2	
9.556E-01	8.419E+01	20	E002	1 0 0 0 2	
7.310E-01	6.441E+01	20	F001	1 0 1 2 2	

(*continued*)

339. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.932E-01	7.870E+01	20	F300	1 0 0 0 2	
8.920E-01	7.860E+01	20	M111	1 0 1 1 2	
7.300E-01	6.432E+01	20	M171	1 0 0 0 1	
7.732E-01	6.812E+01	20	M348	2 2 1 1 2	
9.200E-01	8.106E+01	20	S006	1 0 0 0 1	
8.778E-01	7.734E+01	20.0	K079	1 0 0 0 2	
8.708E-01	7.672E+01	20.40	A016	1 2 1 1 2	
8.417E-01	7.416E+01	25	A016	1 2 1 1 2	
9.084E-01	8.004E+01	25	A094	1 0 0 0 1	
8.243E-01	7.263E+01	25	A326	1 2 0 1 1	
5.396E-02	4.755E+00	25	B004	0 0 0 0 0	*sic*
9.084E-01	8.004E+01	25	B060	2 0 1 1 1	
9.180E-01	8.088E+01	25	B092	2 1 1 1 2	
9.080E-01	8.000E+01	25	B304	2 0 2 2 0	
7.321E-01	6.450E+01	25	C435	0 0 0 0 0	
8.988E-01	7.919E+01	25	D425	0 0 0 0 0	
7.810E-01	6.881E+01	25	G062	1 2 2 2 2	
7.977E-01	7.029E+01	25	L062	2 2 0 1 2	
9.847E-01	8.676E+01	25	L319	1 0 2 1 2	
8.485E-01	7.476E+01	25	M111	1 0 1 1 2	
8.310E-01	7.322E+01	25	P055	1 0 0 0 1	
8.222E-01	7.244E+01	25.0	K079	1 0 0 0 2	
8.436E-01	7.433E+01	25.10	A016	1 2 1 1 2	
7.653E-01	6.743E+01	27.0	G101	1 2 1 1 2	
7.603E-01	6.699E+01	27.5	G101	1 2 1 1 2	
8.124E-01	7.158E+01	30	A016	1 2 1 1 2	
8.115E-01	7.149E+01	30	A016	1 2 1 1 2	
7.524E-01	6.629E+01	30	M088	2 0 0 0 1	
8.124E-01	7.158E+01	30	M111	1 0 1 1 2	
7.524E-01	6.629E+01	30	S357	1 2 1 0 2	
7.889E-01	6.951E+01	30.0	K079	1 0 0 0 2	
7.800E-01	6.873E+01	34	A016	1 2 1 1 2	
7.810E-01	6.881E+01	35	A016	1 2 1 1 2	
7.791E-01	6.864E+01	35	M111	1 0 1 1 2	
8.170E-01	7.198E+01	37	E028	1 0 1 1 2	
7.077E-01	6.235E+01	37	G062	1 2 2 2 2	
7.444E-01	6.559E+01	37.0	K079	1 0 0 0 2	
7.425E-01	6.542E+01	38	J020	2 1 2 1 1	
7.574E-01	6.673E+01	39.90	A016	1 2 1 1 2	
7.504E-01	6.612E+01	40	A016	1 2 1 1 2	
7.395E-01	6.516E+01	40	B108	1 2 0 1 2	
7.524E-01	6.629E+01	40	M111	1 0 1 1 2	
6.696E-01	5.900E+01	40	M348	2 2 1 1 2	
7.278E-01	6.412E+01	40.0	K079	1 0 0 0 2	
6.465E-01	5.696E+01	50	G062	1 2 2 2 2	
6.722E-01	5.923E+01	50.0	K079	1 0 0 0 2	
5.907E-01	5.204E+01	55	M348	2 2 1 1 2	
7.820E-01	6.890E+01	60	B092	2 1 1 1 2	
6.790E-01	5.983E+01	70	A326	1 2 0 1 1	

(*continued*)

339. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.549E-01	4.889E+01	70	M348	2 2 1 1 2	
6.727E-01	5.927E+01	70.4	G101	1 2 1 1 1	
1.156E+00	1.018E+02	.0	K079	1 0 0 0 2	
1.600E-01	1.410E+01	ns	D348	0 0 0 0 0	

340. $C_4H_8O_2$

Methyl propionate
Methylester propanoic acid

RN: 554-12-1 **MP** (°C)**:** –87.0
MW: 88.11 **BP** (°C)**:** 79.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.083E+00	9.545E+01	-2.1	K079	1 0 0 0 2	
1.000E+00	8.811E+01	1.0	K079	1 0 0 0 2	
8.778E-01	7.734E+01	11.5	K079	1 0 0 0 2	
8.500E-01	7.489E+01	14.9	K079	1 0 0 0 2	
8.150E-01	7.181E+01	20	S006	1 0 0 0 2	
8.167E-01	7.195E+01	20.0	K079	1 0 0 0 2	
7.778E-01	6.853E+01	27.1	K079	1 0 0 0 2	
7.667E-01	6.755E+01	32.5	K079	1 0 0 0 2	
7.389E-01	6.510E+01	42.7	K079	1 0 0 0 2	

341. $C_4H_8O_2$

Isobutyric acid
Isobuttersaeure

RN: 79-31-2 **MP** (°C)**:** –47
MW: 88.11 **BP** (°C)**:** 153.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.931E+00	1.701E+02	15.2	P060	1 0 0 0 2	
1.931E+00	1.701E+02	15.2	P060	1 2 0 0 2	
4.171E+00	3.675E+02	17	P060	1 0 0 0 2	
4.171E+00	3.675E+02	17	P060	1 2 0 0 2	
2.619E+00	2.308E+02	17.7	H068	2 0 0 0 1	
1.892E+00	1.667E+02	20	D041	1 0 0 0 0	
1.894E+00	1.669E+02	20	F300	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 2 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 0 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.2	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.25	P060	1 0 0 0 2	
2.367E+00	2.085E+02	20.9	P060	1 0 0 0 2	
2.363E+00	2.082E+02	20.9	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 0 0 0 2	

(*continued*)

341. $C_4H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.161E+00	2.785E+02	21.5	P060	1 2 0 0 2	
3.161E+00	2.785E+02	21.5	P060	1 0 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 2 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 0 0 0 2	
3.240E+00	2.855E+02	21.7	P060	1 2 0 0 2	
3.001E+00	2.644E+02	21.76	P060	1 0 0 0 2	
3.003E+00	2.645E+02	21.79	P060	1 0 0 0 2	
2.831E+00	2.495E+02	21.8	P060	1 2 0 0 2	
2.831E+00	2.495E+02	21.89	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 2 0 0 2	

342. $C_4H_8O_2$

3-Hydroxytetrahydrofuran
(*RS*)-3-Hydroxytetrahydrofuran
Tetrahydro-3-furanol
(±)-3-Hydroxytetrahydrofuran
3-Hydroxyoxolane

RN: 453-20-3 **MP** (°C)**:** <25
MW: 88.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.675E+00	5.000E+02	rt	B066	0 2 0 0 2	

343. $C_4H_8O_2$

Butyric acid
Buttersaeure
n-Butyric acid

RN: 107-92-6 **MP** (°C)**:** –7.9
MW: 88.11 **BP** (°C)**:** 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-02	2.593E+00	1.13	H068	2 0 0 0 1	
1.149E-01	1.012E+01	25	B004	0 0 0 0 0	

344. $C_4H_8O_2$

1,4-Dioxane
1,4-Dioxan
Dioxane

RN: 123-91-1 **MP** (°C)**:** 11.8
MW: 88.11 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>9.08E+00	>8.00E+02	25	B019	1 0 1 2 0	

345. $C_4H_8O_2$

Propyl formate
Ameisensaeure-propylester
Propyl methanoate
n-Propyl formate

RN: 110-74-7 **MP** (°C)**:** –93
MW: 88.11 **BP** (°C)**:** 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.222E-01	3.720E+01	-1.0	K079	1 0 0 0 2	
3.861E-01	3.402E+01	4.0	K079	1 0 0 0 2	
3.722E-01	3.280E+01	6.0	K079	1 0 0 0 2	
3.444E-01	3.035E+01	12.5	K079	1 0 0 0 2	
3.220E-01	2.837E+01	20	S006	1 0 0 0 2	
3.272E-01	2.883E+01	20.0	K079	1 0 0 0 2	
2.497E-01	2.200E+01	22	F300	1 0 0 0 1	
3.161E-01	2.785E+01	30.0	K079	1 0 0 0 2	
2.880E-01	2.537E+01	32.5	N014	0 0 0 0 0	
3.083E-01	2.717E+01	34.0	K079	1 0 0 0 2	
2.972E-01	2.619E+01	45.0	K079	1 0 0 0 2	

346. C_4H_9Br

Isobutyl bromide
1-Bromo-2-methylpropane

RN: 78-77-3 **MP** (°C)**:** –119
MW: 137.03 **BP** (°C)**:** 91.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	5.070E-01	18	F001	1 0 1 0 2	
3.722E-03	5.100E-01	18	F300	1 0 0 0 1	

347. C_4H_9Br

n-Butyl bromide
Bromobutane

RN: 109-65-9 **MP** (°C)**:** –112
MW: 137.03 **BP** (°C)**:** 101.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	5.892E-01	16	F001	1 0 1 0 2	
4.300E-03	5.892E-01	17	S006	1 0 0 0 1	
<1.46E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.500E-03	6.166E-01	25	K012	1 0 0 0 1	
6.340E-03	8.687E-01	25	M342	1 0 1 1 2	
4.434E-03	6.076E-01	30	G029	1 0 2 2 2	
4.500E-02	6.166E+00	ns	H307	0 0 0 0 0	

348. C_4H_9Cl
Isobutyl chloride
Isobutylchlorid
RN: 513-36-0 **MP** (°C)**:** –131
MW: 92.57 **BP** (°C)**:** 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	9.257E-01	12.5	F001	1 0 1 2 2	
9.722E-03	9.000E-01	12.50	F300	2 0 0 0 1	

349. C_4H_9Cl
n-Butyl chloride
1-Chlorobutane
RN: 109-69-3 **MP** (°C)**:** –123.0
MW: 92.57 **BP** (°C)**:** 78.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	6.665E-01	12.5	F001	1 0 1 0 2	
7.130E-02	6.600E+00	12.50	F300	1 0 0 0 1	
8.000E-03	7.406E-01	25	K012	1 0 0 0 0	
9.430E-03	8.729E-01	25	M342	1 0 1 1 2	
7.557E-03	6.995E-01	ns	N034	0 0 0 0 1	

350. C_4H_9Cl
sec-Butyl chloride
2-Chlorobutane
RN: 78-86-4 **MP** (°C)**:** –140
MW: 92.57 **BP** (°C)**:** 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.079E-02	9.990E-01	25	N034	1 0 0 0 0	

351. C_4H_9Cl
tert-Butyl chloride
2-Chloro-2-methylpropane
RN: 507-20-0 **MP** (°C)**:** –26.5
MW: 92.57 **BP** (°C)**:** 51.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.180E-02	7.572E+00	.99	C064	2 2 1 1 2	
6.620E-02	6.128E+00	5.00	C064	2 2 1 1 2	
3.110E-02	2.879E+00	14.90	C064	2 2 1 1 2	

352. C_4H_9I

Iodobutane
n-Butyl iodide
RN: 542-69-8 **MP** (°C)**:** –103
MW: 184.02 **BP** (°C)**:** 130.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.024E-01	17.5	F001	1 0 1 0 2	
1.100E-03	2.024E-01	17.5	S006	1 0 0 0 1	
1.100E-03	2.024E-01	20	M171	1 0 0 0 1	
1.700E-03	3.128E-01	25	K012	1 0 0 0 1	

353. C_4H_9NO

N,N-Dimethylacetamide
Acetdimethylamide
U-5954
RN: 127-19-5 **MP** (°C)**:** –20
MW: 87.12 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E+00	5.289E+02	4.50	C022	1 2 0 0 2	

354. C_4H_9NO

Butyramide
n-Butyramide
RN: 541-35-5 **MP** (°C)**:** 116
MW: 87.12 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E+00	1.708E+02	6	H059	0 0 0 0 0	
2.190E+00	1.908E+02	16	H059	0 0 0 0 0	
2.640E+00	2.300E+02	25	H059	0 0 0 0 0	

355. $C_4H_9NO_2$

γ-Aminobutyric acid
γ-Amino-buttersaeure
γ-Amino-*n*-butyric acid
RN: 56-12-2 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E+01	1.300E+03	25	M029	2 2 2 2 2	

356. $C_4H_9NO_2$
Propyl carbamate
n-Propyl carbamate
RN: 627-12-3 **MP** (°C)**:** 60
MW: 103.12 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E+00	2.001E+02	37	H006	1 2 2 1 2	

357. $C_4H_9NO_2$
DL-α-Aminobutyric acid
DL-2-Aminobutyric acid
RN: 2835-81-6 **MP** (°C)**:** 304
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E+00	2.188E+02	20	D041	1 0 0 0 1	
1.615E+00	1.665E+02	25	K031	2 1 2 1 2	

358. $C_4H_9NO_2$
β-Aminobutyric acid
β-Amino-*n*-butyric acid
RN: 2835-82-7 **MP** (°C)**:** 193
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+01	1.250E+03	25	M029	2 2 2 2 2	

359. $C_4H_9NO_2$
α-Aminoisobutyric acid
α-Amino-isobuttersaeure
α-Aminoisobutyric acid
2-Methylalanine
RN: 62-57-7 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E+00	1.371E+02	25	C018	0 0 0 0 0	
1.170E+00	1.206E+02	25	D041	1 0 0 0 2	
1.482E+00	1.528E+02	25	M029	2 2 2 2 2	
1.759E+00	1.814E+02	25	M097	2 2 2 2 2	

360. $C_4H_9NO_2$
1-Nitrobutane
Butane, 1-nitro-
RN: 627-05-4 **MP** (°C)**:** –81
MW: 103.12 **BP** (°C)**:** 152.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	3.609E+00	25	K012	1 0 0 0 1	

361. $C_4H_9NO_2$
N-Methylurethane
Ethyl methylaminoformate
Ethyl methylcarbamate
Ethyl *N*-methyl carbamate
Methyl urethane
N-Methylurethane
RN: 105-40-8 **MP** (°C)**:**
MW: 103.12 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.97E+00	+4.10E+02	ns	S460	0 0 0 0 0	

362. $C_4H_9NO_2$
α-Aminobutyric acid
2-Aminobutanoic acid
α-Amino-n-butyric acid
Butanoic acid
RN: 80-60-4 **MP** (°C)**:** 304
MW: 103.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	1.902E+02	25	A048	1 1 1 1 2	form A
1.624E+00	1.674E+02	25	A048	1 1 1 1 2	form B
1.800E+00	1.856E+02	25	C018	0 0 0 0 0	
1.800E+00	1.856E+02	25	E015	1 2 1 1 2	
2.041E+00	2.105E+02	25	M029	2 2 2 2 2	
1.852E+00	1.910E+02	35	A048	1 1 1 1 2	form A
1.771E+00	1.826E+02	35	A048	1 1 1 1 2	form B
1.931E+00	1.991E+02	45	A048	1 1 1 1 2	form A
1.917E+00	1.977E+02	45	A048	1 1 1 1 2	form B

363. $C_4H_9NO_3$
L-Threonine
Threonine
RN: 72-19-5 **MP** (°C)**:** 270
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.606E-01	9.060E+01	20	B032	1 2 2 1 2	
8.139E-01	9.695E+01	25	B032	1 2 2 1 2	
7.346E-01	8.751E+01	25	G315	0 0 0 0 0	
8.202E-01	9.770E+01	25.1	N024	0 0 0 0 0	
8.227E-01	9.800E+01	25.1	N026	0 0 0 0 0	
7.493E-01	8.925E+01	25.1	N027	1 1 2 2 2	
8.168E-01	9.730E+01	27	D036	0 0 0 0 0	
8.695E-01	1.036E+02	29.80	B032	1 2 2 1 2	

364. $C_4H_9NO_3$
DL-*allo*-Threonine
DL-Allothreonine
RN: 144-98-9 **MP** (°C)**:**
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E+00	1.220E+02	25	D041	1 0 0 0 2	
1.987E+00	2.366E+02	80	D041	1 0 0 0 2	

365. $C_4H_9NO_3$
DL-Threonine
(±)-Threonine
RN: 80-68-2 **MP** (°C)**:** 244
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E+00	1.674E+02	25	D041	1 0 0 0 2	
2.979E+00	3.548E+02	80	D041	1 0 0 0 1	

366. $C_4H_9NO_3$
Butyl nitrate
N-Butyl nitrate
RN: 928-45-0 **MP** (°C)**:**
MW: 119.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-03	7.743E-01	25	K012	1 0 0 0 1	

367. $C_4H_9N_3O_2$
Creatine
Kreatin
RN: 57-00-1 **MP** (°C)**:** 219
MW: 131.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.222E-02	1.078E+01	10	D041	1 0 0 0 2	
1.016E-01	1.332E+01	18	D041	1 0 0 0 2	
1.014E-01	1.330E+01	18	F300	1 0 0 0 2	

368. $C_4H_9O_5P$
γ-Phosphono-*n*-butyric acid
4-Phosphonobutyric acid
Phosphonic acid, (3-carboxypropyl)-
Butyric acid, 4-phosphono-
RN: 4378-43-2 **MP** (°C)**:**
MW: 168.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E+00	2.923E+02	0	N028	1 0 0 0 2	
2.068E+00	3.477E+02	20	N028	1 0 0 0 2	

369. C_4H_{10}
Isobutane
1,1-Dimethylethane
2-Methylpropane
Trimethylmethane
Purifrigor iso 3.5
R 600α
RN: 75-28-5 **MP** (°C)**:** –159
MW: 58.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~5.68E-03	~3.30E-01	17	F300	1 0 0 0 0	
8.413E-04	4.890E-02	25	M001	2 1 2 2 2	
8.413E-04	4.890E-02	25	M002	2 1 2 2 2	

370. C_4H_{10}

Butane
n-Butane
Diethyl
HC 600
Liquefied petroleum gas
R 600 (alkane)

RN: 106-97-8 **MP** (°C)**:** –138
MW: 58.12 **BP** (°C)**:** –0.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	1.824E-01	3	R063	0 0 0 0 0	
3.210E-03	1.866E-01	4	K031	2 1 2 1 2	
2.622E-03	1.524E-01	6	R063	0 0 0 0 0	
2.314E-03	1.345E-01	9	R063	0 0 0 0 0	
1.886E-03	1.096E-01	14	R063	0 0 0 0 0	
1.461E-03	8.492E-02	19.8	G058	1 0 0 0 2	
1.260E-03	7.324E-02	25	K031	2 1 2 1 2	
1.056E-03	6.140E-02	25	M001	2 1 2 2 2	
1.056E-03	6.140E-02	25	M002	2 1 2 2 2	
1.056E-03	6.140E-02	25	M040	1 0 0 1 2	
2.773E-02	1.612E+00	38	R078	0 0 0 0 0	
6.600E-04	3.836E-02	50	K031	2 1 2 1 2	
1.159E-01	6.735E+00	71	R078	0 0 0 0 0	
4.596E-01	2.671E+01	104	R078	0 0 0 0 0	
1.370E+00	7.965E+01	138	R078	0 0 0 0 0	

371. $C_4H_{10}NO_3PS$

Acephate
Orthene
Acetylphosphoramidothioic acid *O,S*-dimethyl ester

RN: 30560-19-1 **MP** (°C)**:** 85.5
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E+00	3.939E+02	rt	M161	0 0 0 0 1	

372. $C_4H_{10}N_2O$

N-Nitrosodiethylamine
Diethyl nitrosamine

RN: 55-18-5 **MP** (°C)**:**
MW: 102.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.062E+02	24	D083	2 0 0 0 2	

373. $C_4H_{10}O$

Methyl propyl ether
1-Methoxypropane

RN: 557-17-5 **MP** (°C)**:** <25
MW: 74.12 **BP** (°C)**:** 38.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.154E-01	5.303E+01	0	B002	2 1 1 2 2	
4.939E-01	3.661E+01	10	B002	2 1 1 2 2	
4.436E-01	3.288E+01	15	B002	2 1 1 2 2	
4.183E-01	3.101E+01	20	B002	2 1 1 2 2	
3.993E-01	2.960E+01	25	B002	2 1 1 2 2	

374. $C_4H_{10}O$

tert-Butyl alcohol
2-Methyl-2-propanol
tert-Butanol

RN: 75-65-0 **MP** (°C)**:** 25.6
MW: 74.12 **BP** (°C)**:** 82.41

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.712E-02	6.458E+00	79.40	B165	1 0 1 1 2	

375. $C_4H_{10}O$

n-Butyl alcohol
Butanol-(1)
n-Butanol
1-Butanol
Butyl alcohol
n-Butyl alcohol

RN: 71-36-3 **MP** (°C)**:** –90
MW: 74.12 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E+00	9.355E+01	0	E029	1 2 0 1 2	
1.176E+00	8.717E+01	0	M095	2 2 1 2 2	
1.176E+00	8.717E+01	5	H003	1 2 1 1 2	
1.077E+00	7.987E+01	10	E029	1 2 0 1 2	
1.104E+00	8.181E+01	10	H003	1 2 1 1 2	
6.015E+00	4.459E+02	13.0	J012	1 2 0 1 2	
1.024E+00	7.587E+01	15	H003	1 2 1 1 2	
1.034E+00	7.664E+01	15	M095	2 2 1 2 2	
9.190E-01	6.812E+01	18	F001	1 0 1 0 2	
8.634E-01	6.400E+01	18	F300	1 0 0 0 1	
7.396E-01	5.482E+01	20	A075	1 0 0 0 1	
9.762E-01	7.236E+01	20	D040	2 2 1 1 2	

(*continued*)

375. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.993E-01	7.407E+01	20	D052	1 1 0 0 0	
9.482E-01	7.029E+01	20	E029	1 2 0 1 2	
9.773E-01	7.244E+01	20	H003	1 2 1 1 2	
6.302E-01	4.671E+01	20	L084	1 1 1 1 1	
1.040E+00	7.709E+01	20	M312	1 0 0 0 1	
8.270E-01	6.130E+01	23	D063	1 0 1 2 2	
1.021E+00	7.567E+01	23.5	D063	1 0 0 2 2	
9.983E-01	7.400E+01	25	A049	1 0 1 0 0	
1.125E+00	8.341E+01	25	B019	1 0 1 2 0	
9.645E-01	7.149E+01	25	B060	2 0 1 1 1	
1.000E+00	7.412E+01	25	F044	1 0 0 0 0	EFG
8.708E-01	6.455E+01	25	F325	1 2 0 1 1	
9.200E-01	6.819E+01	25	G075	1 0 1 0 1	
9.237E-01	6.847E+01	25	H003	1 2 1 1 2	
9.307E-01	6.899E+01	25	H028	2 0 2 0 2	
1.070E+00	7.931E+01	25	K012	1 0 0 0 2	
9.700E-01	7.190E+01	25	K025	2 2 1 1 1	
8.867E-01	6.572E+01	25	L322	1 1 2 2 1	
8.904E-01	6.600E+01	25	M136	2 0 0 0 1	
8.904E-01	6.600E+01	25	M139	2 0 0 0 1	
8.826E-01	6.542E+01	25.0	P077	1 1 1 1 1	
8.234E-01	6.103E+01	26	O012	1 2 1 1 2	
8.826E-01	6.542E+01	27	R319	2 2 2 1 1	
5.976E+00	4.429E+02	29.82	J012	1 2 0 1 2	
8.944E-01	6.629E+01	30	D040	2 2 1 1 2	
8.897E-01	6.594E+01	30	E029	1 2 0 1 2	
8.920E-01	6.612E+01	30	F053	1 0 2 0 2	
8.920E-01	6.612E+01	30	H003	1 2 1 1 2	
8.838E-01	6.551E+01	30.0	H043	2 2 1 1 2	
8.625E-01	6.393E+01	35	H003	1 2 1 1 2	
9.061E-01	6.716E+01	38	J020	2 0 2 1 1	
8.471E-01	6.279E+01	38	M125	1 1 1 1 1	
5.933E-01	4.398E+01	40	A075	1 0 0 0 1	
8.353E-01	6.191E+01	40	D040	2 2 1 1 2	
8.495E-01	6.297E+01	40	E029	1 2 0 1 2	
8.353E-01	6.191E+01	40	H003	1 2 1 1 2	
8.234E-01	6.103E+01	45	M095	2 2 1 2 2	
8.293E-01	6.147E+01	50	E029	1 2 0 1 2	
8.186E-01	6.068E+01	50	H003	1 2 1 1 2	
7.756E-01	5.749E+01	50	O012	1 2 1 1 2	
5.837E+00	4.327E+02	58.50	J012	1 2 0 1 2	
5.064E-01	3.754E+01	60	A075	1 0 0 0 1	
8.258E-01	6.121E+01	60	E029	1 2 0 1 2	
8.258E-01	6.121E+01	60	H003	1 2 1 1 2	
5.064E-01	3.754E+01	70	A075	1 0 0 0 1	
8.436E-01	6.253E+01	70	E029	1 2 0 1 2	
8.850E-01	6.560E+01	70	F001	1 0 1 0 2	
8.507E-01	6.306E+01	70	H003	1 2 1 1 2	

(*continued*)

375. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-01	4.943E+01	75	L084	1 1 1 1 1	
8.590E-01	6.367E+01	75	M095	2 2 1 2 1	
8.708E-01	6.455E+01	80	E029	1 2 0 1 2	
9.460E-01	7.012E+01	80	F001	1 0 1 0 2	
8.696E-01	6.446E+01	80	H003	1 2 1 1 2	
9.412E-01	6.977E+01	90	E029	1 2 0 1 2	
1.054E+00	7.813E+01	90	F001	1 0 1 0 2	
9.762E-01	7.236E+01	90	M095	2 2 1 2 1	
1.084E+00	8.038E+01	97.90	H003	1 2 1 1 2	
1.101E+00	8.164E+01	98.3	R072	2 2 2 1 2	
4.900E+00	3.632E+02	100	E029	1 2 0 1 2	
1.228E+00	9.102E+01	100	F001	1 0 1 0 2	
1.204E+00	8.925E+01	105	M095	2 2 1 2 1	
1.342E+00	9.950E+01	110	E029	1 2 0 1 2	
1.473E+00	1.092E+02	110	F001	1 0 1 0 2	
1.523E+00	1.129E+02	114.50	H003	1 2 1 1 2	
1.600E+00	1.186E+02	116.90	H003	1 2 1 1 2	
1.805E+00	1.338E+02	120	E029	1 2 0 1 2	
2.223E+00	1.648E+02	123.30	H003	1 2 1 1 2	
2.890E+00	2.142E+02	124.80	H003	1 2 1 1 2	
2.567E+00	1.903E+02	125	E029	1 2 0 1 2	
3.334E+00	2.471E+02	125.10	H003	1 2 1 1 2	
3.148E+00	2.334E+02	125.20	H003	1 2 1 1 2	
9.307E-01	6.899E+01	ns	A406	0 0 0 0 1	
7.920E-01	5.871E+01	ns	D348	0 0 0 0 0	
9.744E-01	7.222E+01	ns	L003	0 0 2 1 2	
9.033E+00	6.695E+02	ns	M314	2 1 2 1 2	

376. $C_4H_{10}O$

Methyl isopropyl ether
2-Methoxypropane

RN: 598-53-8 **MP** (°C)**:** <25
MW: 74.12 **BP** (°C)**:** 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E+00	8.842E+01	10	B002	2 1 1 2 2	
1.068E+00	7.919E+01	15	B002	2 1 1 2 2	
9.295E-01	6.890E+01	20	B002	2 1 1 2 2	
8.234E-01	6.103E+01	25	B002	2 1 1 2 2	
8.437E-01	6.254E+01	ns	J300	0 0 0 0 0	

377. $C_4H_{10}O$

Isobutyl alcohol
2-Methyl-1-propanol

RN: 78-83-1 **MP** (°C)**:** –108
MW: 74.12 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E+00	1.001E+02	18	F001	1 0 1 2 2	
1.228E+00	9.100E+01	18	F300	1 0 0 0 0	
1.278E+00	9.471E+01	20	M146	1 2 2 2 2	
1.280E+00	9.488E+01	20	M312	1 0 0 0 1	
1.000E+00	7.416E+01	25	A037	2 2 2 2 2	
1.226E+00	9.091E+01	25	D052	1 1 0 0 2	
9.529E-01	7.063E+01	25	F050	1 0 0 0 1	
8.967E-01	6.647E+01	25	F317	2 1 1 1 2	
1.045E+00	7.749E+01	29.84	M114	2 2 1 1 1	
9.529E-01	7.063E+01	39.74	M114	2 2 1 1 1	
8.234E-01	6.103E+01	49.64	M114	2 2 1 1 1	
8.590E-01	6.367E+01	59.54	M114	2 2 1 1 1	
9.295E-01	6.890E+01	79.24	M114	2 2 1 1 1	
9.645E-01	7.149E+01	89.14	M114	2 2 1 1 1	
5.168E+00	3.831E+02	90.5	J017	1 0 1 2 2	
5.033E+00	3.730E+02	91.0	J017	1 0 1 2 2	
4.887E+00	3.622E+02	92.0	J017	1 0 1 2 2	
4.871E+00	3.610E+02	92.1	J017	1 0 1 2 2	
4.615E+00	3.421E+02	93.0	J017	1 0 1 2 2	
4.135E+00	3.065E+02	94.3	J017	1 0 1 2 2	
3.820E+00	2.832E+02	95.3	J017	1 0 1 2 2	
1.215E+00	9.008E+01	99.04	M114	2 2 1 1 1	
1.348E+00	9.991E+01	108.94	M114	2 2 1 1 2	
1.708E+00	1.266E+02	118.74	M114	2 2 1 1 2	
2.009E+00	1.489E+02	123.74	M114	2 2 1 1 2	
2.239E+00	1.660E+02	125.64	M114	2 2 1 1 2	
2.415E+00	1.790E+02	128.64	M114	2 2 1 1 2	
2.637E+00	1.955E+02	130.64	M114	2 2 1 1 2	
3.000E+00	2.224E+02	132.64	M114	2 2 1 1 2	
3.527E+00	2.614E+02	134.14	M114	2 2 1 1 2	
1.179E+00	8.740E+01	ns	L003	0 0 2 1 1	

378. $C_4H_{10}O$

Ethyl ether
Diaethylaether
Diethyl ether

RN: 60-29-7 **MP** (°C)**:** –116
MW: 74.12 **BP** (°C)**:** 34.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E+00	1.131E+02	–3.8	H002	2 0 0 1 2	
1.410E+00	1.045E+02	0	H002	1 0 0 1 2	
1.662E+00	1.232E+02	0	K077	1 2 2 2 2	average of 3
1.338E+00	9.920E+01	7.5	K077	1 2 2 2 2	

(*continued*)

378. $C_4H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.263E+00	9.360E+01	8.5	K077	1 2 2 2 2	
1.118E+00	8.291E+01	10	H002	1 0 0 1 2	
1.115E+00	8.265E+01	10	K002	1 2 1 1 2	
1.105E+00	8.190E+01	12	K077	1 2 2 2 2	
9.796E-01	7.261E+01	15	F055	1 2 2 2 2	
1.133E+00	8.400E+01	15	F300	1 0 0 0 1	
9.893E-01	7.333E+01	15	H002	1 0 0 1 2	
9.843E-01	7.296E+01	15	K002	1 2 1 1 2	
8.430E+00	6.249E+02	15	M069	1 0 0 0 2	
1.137E+00	8.430E+01	15	T033	1 2 1 1 2	
1.029E+00	7.630E+01	16	K077	1 2 2 2 2	
8.837E-01	6.550E+01	19	K077	1 2 2 2 2	average
8.696E-01	6.446E+01	20	F055	1 2 2 2 2	
8.703E-01	6.451E+01	20	H002	1 0 0 1 2	
8.684E-01	6.437E+01	20	K002	1 2 1 1 2	
8.353E-01	6.191E+01	20	M345	2 1 1 1 1	
8.341E-01	6.183E+01	20	N038	1 0 0 1 2	
8.769E-03	6.500E-01	21	H337	1 0 1 0 2	*sic*
1.012E+00	7.502E+01	22	H072	1 0 1 1 2	
9.993E-01	7.407E+01	25	B019	1 0 1 2 0	
7.636E-01	5.660E+01	25	F055	1 2 2 2 2	
8.095E-01	6.000E+01	25	F300	1 0 0 0 1	
7.669E-01	5.684E+01	25	H002	1 0 0 1 2	
7.684E-01	5.696E+01	25	K002	1 2 1 1 2	
8.800E-01	6.523E+01	25	K012	1 0 0 0 1	
6.050E+00	4.484E+02	25	M069	1 0 0 0 2	
8.471E-01	6.279E+01	25	M345	2 1 1 1 1	
8.162E-01	6.050E+01	25	T033	1 2 1 1 2	
1.048E-02	7.770E-01	26	H337	1 0 1 0 2	*sic*
6.839E-01	5.069E+01	30	H002	1 0 0 1 2	
6.839E-01	5.069E+01	30	K002	1 2 1 1 2	
6.799E-01	5.040E+01	30	K077	1 2 2 2 2	
1.073E-02	7.950E-01	32	H337	1 0 1 0 2	*sic*
5.950E-01	4.410E+01	37	E022	1 0 1 1 0	
7.120E-01	5.278E+01	37	E028	1 0 1 1 2	
9.484E-03	7.030E-01	37	H337	1 0 1 0 2	*sic*
6.314E-01	4.680E+01	38	K077	1 2 2 2 2	
9.417E-03	6.980E-01	38.5	H337	1 0 1 0 2	*sic*
9.808E-03	7.270E-01	40	H337	1 0 1 0 2	*sic*
5.545E-01	4.110E+01	49	K077	1 2 2 2 2	
5.491E-01	4.070E+01	51.5	K077	1 2 2 2 2	
4.857E-01	3.600E+01	62.5	K077	1 2 2 2 2	
4.600E-01	3.410E+01	65	K077	1 2 2 2 2	
4.209E-01	3.120E+01	66.5	K077	1 2 2 2 2	
4.020E-01	2.980E+01	71	K077	1 2 2 2 2	
3.912E-01	2.900E+01	72	K077	1 2 2 2 2	
3.643E-01	2.700E+01	82	K077	1 2 2 2 2	
1.770E-01	1.312E+01	ns	D348	0 0 0 0 0	
9.412E-01	6.977E+01	ns	R028	0 0 0 0 0	
8.826E-01	6.542E+01	rt	B066	0 2 0 0 0	

379. $C_4H_{10}O$

sec-Butyl alcohol
DL-*sec*-Butyl alcohol
DL-Butanol-(2)
sec-DL-Butyl alcohol

RN: 78-92-2 **MP** (°C)**:** –114
MW: 74.12 **BP** (°C)**:** 99.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	1.929E+02	10.04	M119	2 2 2 2 2	
3.222E+00	2.388E+02	20	A070	1 2 1 0 2	
1.499E+00	1.111E+02	20	D052	1 1 0 0 0	
2.106E+00	1.561E+02	20	E019	1 0 1 1 2	
1.497E+00	1.110E+02	20	F300	1 0 0 0 2	
2.230E+00	1.653E+02	20	M112	2 2 1 1 2	
2.267E+00	1.681E+02	20.04	M119	2 2 2 2 2	
1.348E+00	9.991E+01	25	B019	1 0 1 2 0	
1.057E+00	7.834E+01	25	B060	2 0 1 1 1	
1.699E+00	1.260E+02	25	B165	1 0 1 1 1	
2.048E+00	1.518E+02	27.04	M119	2 2 2 2 2	
2.556E+00	1.894E+02	40	A070	1 2 1 0 2	
1.821E+00	1.349E+02	40	M112	2 0 1 1 2	
1.749E+00	1.297E+02	40.04	M119	2 2 2 2 2	
1.573E+00	1.166E+02	50.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	60	A070	1 2 1 0 2	
1.657E+00	1.228E+02	60	M112	2 0 1 1 2	
1.531E+00	1.135E+02	60.04	M119	2 2 2 2 2	
1.541E+00	1.143E+02	70.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	80	A070	1 2 1 0 2	
1.657E+00	1.228E+02	80	M112	2 0 1 1 2	
1.636E+00	1.213E+02	80.04	M119	2 2 2 2 2	
1.760E+00	1.304E+02	85	M112	2 0 1 1 2	
5.107E-02	3.786E+00	87.30	B165	1 0 1 1 2	
1.810E+00	1.342E+02	90.04	M119	2 2 2 2 2	
2.087E+00	1.547E+02	100.04	M119	2 2 2 2 2	
2.602E+00	1.929E+02	110.04	M119	2 2 2 2 2	
1.901E+00	1.409E+02	ns	L003	0 0 2 1 2	

380. $C_4H_{10}O_2S$

Diethyl sulfone
Diaethylsulfon

RN: 597-35-3 **MP** (°C)**:** 73
MW: 122.19 **BP** (°C)**:** 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E+00	1.350E+02	16	F300	1 0 0 0 2	

381. $C_4H_{10}O_4$
DL-Threitol
DL-1,2,3,4-Butanetetrol
RN: 6968-16-7 **MP** (°C)**:** 90
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.353E+00	8.980E+02	25	C346	0 0 0 0 0	

382. $C_4H_{10}O_4$
Erythritol
Erythrit
RN: 149-32-6 **MP** (°C)**:** 121.5
MW: 122.12 **BP** (°C)**:** 330

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.118E+00	3.808E+02	rt	D021	0 0 1 1 2	
4.995E+00	6.100E+02	rt	F300	0 0 0 0 2	

383. $C_4H_{10}S$
Ethyl sulfide
1,1′-Thiobisethane
Diethyl thioether
RN: 352-93-2 **MP** (°C)**:** –100
MW: 90.19 **BP** (°C)**:** 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	3.066E+00	25	K012	1 0 0 0 1	

384. $C_4H_{11}N$
sec-Butylamine
DL-*sec*-Butylamine
DL-*sec*-Butylamin
RN: 13952-84-6 **MP** (°C)**:**
MW: 73.14 **BP** (°C)**:** 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+00	1.120E+02	20	F300	1 0 0 0 2	

385. $C_4H_{11}N$

n-Butylamine
n-Butylamin
1-Aminobutane
RN: 109-73-9 **MP** (°C)**:** –50
MW: 73.14 **BP** (°C)**:** 78

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-02	2.384E+00	25	B004	0 0 0 0 0	

386. $C_4H_{11}NO_3$

Tromethamine
tris-(Hydroxymethyl)-amino-methan
tris-(Hydroxymethyl)-aminomethane
2-Amino-2-(hydroxymethyl)-1,3-propanediol
tris(Hydroxymethyl)methylamine
RN: 77-86-1 **MP** (°C)**:** 171.5
MW: 121.14 **BP** (°C)**:** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.564E+00	5.529E+02	15	E305	0 0 0 0 0	
5.766E+00	6.985E+02	25	E305	0 0 0 0 0	
7.160E+00	8.673E+02	35	E305	0 0 0 0 0	

387. $C_4H_{11}NO_8P_2$

Glyphosine
Polaris
N,*N*-bis(Phosphonomethyl)glycine
RN: 2439-99-8 **MP** (°C)**:**
MW: 263.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.427E-01	2.480E+02	20	M161	1 0 0 0 2	

388. C_4Cl_6

Hexachloro-1,3-butadiene
Hexachlorobutadiene
RN: 87-68-3 **MP** (°C)**:** –19
MW: 260.76 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	2.548E-03	20	C113	1 0 2 1 2	
1.917E-05	5.000E-03	20	M068	1 0 0 0 0	
~7.67E-06	~2.00E-03	20	M133	1 0 0 0 0	
1.240E-05	3.233E-03	25	B173	2 0 2 2 2	
7.668E-04	2.000E-01	ns	M061	0 0 0 0 1	

389. $C_5H_2Cl_3NO$
2,3,5-Trichloro-4-hydroxypyridine
Daxtrom
RN: 1970-40-7 **MP** (°C)**:** 216
MW: 198.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.871E-03	5.697E-01	25	M061	1 0 0 0 1	

390. $C_5H_2Cl_3NO$
3,5,6-Trichloro-2-pyridinol
3,5,6-Trichloropyridinol
Hydroxy-3,5,6-trichloropyridine
Pyridinone, 3,5,6-trichloro-
RN: 6515-38-4 **MP** (°C)**:**
MW: 198.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.200E-01	26.70	L095	2 2 1 1 2	
1.109E-03	2.200E-01	ns	K138	0 0 0 0 1	

391. $C_5H_3F_3N_2O_2$
5-Trifluoromethyl uracil
Trifluorothymine
RN: 54-20-6 **MP** (°C)**:**
MW: 180.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.451E-01	2.613E+01	25	S471	0 0 0 0 0	
1.492E-01	2.687E+01	25	S471	0 0 0 0 0	

392. $C_5H_4ClN_5$
2-Chloroadenine
1H-Purin-6-amine, 2-chloro-
6-Amino-2-chloropurine
2-Chloro-6-aminopurine
SQ 22982
RN: 1839-18-5 **MP** (°C)**:**
MW: 169.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-05	8.300E-03	25	A336	0 0 0 0 0	

393. $C_5H_4N_2O_4$
Orotic acid
Vitamin B13
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid
RN: 65-86-1 **MP** (°C)**:** 345.5
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-02	1.815E+00	18	B135	1 0 0 0 0	

394. $C_5H_4N_2O_4$
α,β-Imidazoledicarboxylic acid
4,5-Imidazoledicarboxylic acid
Imidazol-di-carbonsaeure-(4,5)
RN: 570-22-9 **MP** (°C)**:** 288
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.203E-03	5.000E-01	20	F300	1 0 0 0 1	
8.328E-03	1.300E+00	100	F300	1 0 0 0 1	

395. $C_5H_4N_2O_4$
5-Carboxyuracil
5-Uracilcarboxylic acid
2,4-Dihydroxypyrimidine-5-carboxylic acid
Uracil-carbonsaeure-(4)
RN: 23945-44-0 **MP** (°C)**:** 283
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	1.800E+00	20	F300	1 0 0 0 1	
7.000E-03	1.093E+00	20	N019	0 0 0 0 0	

396. $C_5H_4N_4$
Purine
7-Imidazo(4,5-d)pyrimidine
RN: 120-73-0 **MP** (°C)**:** 216
MW: 120.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.775E+00	3.333E+02	20	A018	1 0 1 1 0	
2.754E+00	3.308E+02	ns	R427	0 0 0 0 0	

397. $C_5H_4N_4O$
Hypoxanthine
Hypoxanthin
RN: 68-94-0 **MP** (°C)**:** 150dec
MW: 136.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-03	6.995E-01	19	D041	1 0 0 0 0	
5.143E-03	7.000E-01	23	F300	1 0 0 0 1	
5.290E-03	7.200E-01	25	A337	0 0 0 0 0	
~1.90E-03	~2.59E-01	39.99	T420	0 0 0 0 0	
1.042E-01	1.418E+01	100	D004	0 0 0 0 0	
1.080E-01	1.470E+01	100	F300	1 0 0 0 2	
5.359E-03	7.294E-01	c	D004	0 0 0 0 0	

398. $C_5H_4N_4O$
Allopurinol
1H-Pyrazolo(3,4-d)pyrimidin-4-ol
Lopurin
RN: 315-30-0 **MP** (°C)**:** >350
MW: 136.11 **BP** (°C)**:** 559.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-03	3.450E-01	15	C095	1 0 0 1 2	
3.673E-03	5.000E-01	22	B322	0 0 0 0 0	
3.673E-03	5.000E-01	22	B428	1 2 1 2 1	
3.526E-03	4.800E-01	25	B189	1 0 0 0 1	
4.180E-03	5.690E-01	25	C095	1 0 0 1 2	
6.502E-03	8.850E-01	35	C095	1 0 0 1 2	
7.964E-03	1.084E+00	40	C095	1 0 0 1 2	
3.526E-03	4.800E-01	ns	A351	0 0 0 0 0	
2.475E-03	3.369E-01	ns	B404	0 2 1 1 0	
5.730E-03	7.800E-01	ns	H067	0 0 0 0 0	
7.347E-04	1.000E-01	ns	K444	0 0 0 0 0	

399. $C_5H_4N_4O$
8-Hydroxypurine
9H-Purin-8-ol
RN: 51953-05-0 **MP** (°C)**:**
MW: 136.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.048E-02	4.149E+00	20	A022	1 0 0 0 0	

400. $C_5H_4N_4O_2$
Xanthine
2,6-Dioxopurine
1H-Purine-2,6-dione, 3,7-dihydro-
RN: 69-89-6 **MP** (°C)**:** >300
MW: 152.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.285E-03	4.998E-01	20	D041	1 0 0 0 0	
3.000E-04	4.563E-02	20.99	T418	0 0 0 0 0	
2.458E-04	3.739E-02	21	L015	1 0 1 1 2	
5.246E-04	7.980E-02	37	L015	1 0 1 1 2	
1.312E-02	1.996E+00	100	D041	1 0 0 0 0	

401. $C_5H_4N_4O_2.H_2O$
Xanthine (monohydrate)
RN: 69-89-6 **MP** (°C)**:** >150dec
MW: 170.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.082E-04	6.944E-02	c	D004	0 0 0 0 0	
3.916E-03	6.662E-01	h	D004	0 0 0 0 0	

402. $C_5H_4N_4O_3$
Uric acid
Harnsaeure
RN: 69-93-2 **MP** (°C)**:**
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-04	2.000E-02	0	M043	1 0 0 0 0	
7.110E-05	1.195E-02	2.6	M315	1 0 1 1 2	
1.029E-04	1.730E-02	5	R042	1 2 2 1 2	
1.050E-04	1.765E-02	9.3	M315	1 0 1 1 2	
2.379E-04	4.000E-02	10	M043	1 0 0 0 0	
1.326E-04	2.230E-02	14	B116	2 0 1 1 2	
1.190E-04	2.000E-02	20	D041	1 0 0 0 0	
3.569E-04	6.000E-02	20	M043	1 0 0 0 0	
6.610E-04	1.111E-01	22	M145	1 0 1 2 2	intrinsic
1.862E-04	3.130E-02	25	R042	1 2 2 1 2	
2.070E-04	3.480E-02	25.0	M315	1 0 1 1 2	
5.354E-04	9.000E-02	30	F300	1 0 0 0 2	
5.353E-04	8.999E-02	30	M043	1 0 0 0 0	
3.660E-04	6.153E-02	37.0	M315	1 0 1 1 2	
7.137E-04	1.200E-01	40	M043	1 0 0 0 1	
3.753E-04	6.310E-02	40	R042	1 2 2 1 2	
6.280E-04	1.056E-01	50.0	M315	1 0 1 1 2	
6.960E-04	1.170E-01	54	R042	1 2 2 1 2	
1.368E-03	2.299E-01	60	M043	1 0 0 0 1	

(*continued*)

402. $C_5H_4N_4O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-03	2.450E-01	70	F300	1 0 0 0 2	
2.319E-03	3.898E-01	80	M043	1 0 0 0 1	
2.974E-04	5.000E-02	100	D041	1 0 0 0 0	
4.961E-03	8.340E-01	100	F300	1 0 0 0 0	
3.686E-03	6.196E-01	100	M043	1 0 0 0 1	

403. $C_5H_4N_4O_3.2H_2O$

Uric acid (dihydrate)

RN: 69-93-2 **MP** (°C)**:**
MW: 204.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.620E-05	1.964E-02	2.6	M315	1 0 1 1 2	
1.420E-04	2.899E-02	9.3	M315	1 0 1 1 2	
3.390E-04	6.920E-02	25.0	M315	1 0 1 1 2	
6.560E-04	1.339E-01	37.0	M315	1 0 1 1 2	
1.440E-03	2.940E-01	50.0	M315	1 0 1 1 2	

404. $C_5H_4N_4S$

6-Mercaptopurine
6-Purinethiol
Mercaptopurine
Purine-6-thiol
Leukeran

RN: 50-44-2 **MP** (°C)**:**
MW: 152.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	4.565E-02	4.62	A034	1 1 2 2 0	EFG
8.148E-04	1.240E-01	25	N063	1 1 1 1 2	
4.500E-02	6.848E+00	29.87	A034	1 1 2 2 1	EFG
1.703E-03	2.591E-01	37	H046	1 1 1 1 2	
2.658E-03	4.045E-01	ns	N050	0 1 1 0 0	

405. $C_5H_4O_2$

Furfural
2-Furaldehyde
Furfurol

RN: 98-01-1 **MP** (°C)**:** –36
MW: 96.09 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.620E-01	7.322E+01	10	M099	1 2 0 1 1	
7.816E-01	7.510E+01	16	M099	1 2 0 1 2	
7.869E-01	7.561E+01	17	M099	1 2 0 1 2	
7.976E-01	7.664E+01	20	D052	1 1 0 0 0	

(*continued*)

405. $C_5H_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.972E-01	7.660E+01	20	F300	1 0 0 0 2	
7.976E-01	7.664E+01	20	M099	1 2 0 1 1	
7.620E-01	7.322E+01	25	C056	1 2 1 1 1	
8.197E-01	7.877E+01	25	C329	1 2 1 1 1	average
7.709E-01	7.407E+01	25	H338	2 2 1 2 2	
7.976E-01	7.664E+01	25	H340	0 0 0 0 0	
7.441E-01	7.149E+01	25	L062	2 2 1 2 1	
7.709E-01	7.407E+01	25	L320	2 2 1 2 1	
8.242E-01	7.919E+01	25	M099	1 2 0 1 1	
8.347E-01	8.021E+01	27	M099	1 2 0 1 2	
8.347E-01	8.021E+01	27.20	M099	1 2 0 1 2	
8.312E-01	7.987E+01	27.50	M099	1 2 0 1 2	
8.418E-01	8.088E+01	30	M099	1 2 0 1 1	
8.488E-01	8.156E+01	35	H338	2 2 1 2 2	
8.506E-01	8.173E+01	35	L320	2 2 1 2 1	
9.029E-01	8.676E+01	38	G050	1 0 2 1 1	
8.619E-01	8.282E+01	39.50	E037	1 2 2 2 2	
9.029E-01	8.676E+01	40	M099	1 2 0 1 1	
9.289E-01	8.925E+01	44	M099	1 2 0 1 2	
9.804E-01	9.420E+01	50	M099	1 2 0 1 2	
1.023E+00	9.829E+01	52	G050	1 0 2 1 2	
9.306E-01	8.942E+01	53.10	E037	1 2 2 2 2	
4.982E+00	4.787E+02	53.30	E037	1 2 2 2 2	
1.090E+00	1.047E+02	60	M099	1 2 0 1 2	
1.107E+00	1.063E+02	61	M099	1 2 0 1 2	
1.156E+00	1.111E+02	66	G050	1 0 2 1 2	
1.156E+00	1.111E+02	66	M099	1 2 0 1 2	
1.214E+00	1.166E+02	70	M099	1 2 0 1 2	
4.895E+00	4.703E+02	73.60	E037	1 2 2 2 2	
1.318E+00	1.266E+02	79	G050	1 0 2 1 2	
1.342E+00	1.289E+02	80	M099	1 2 0 1 2	
1.361E+00	1.307E+02	85.80	E037	1 2 2 2 2	
1.482E+00	1.424E+02	90	M099	1 2 0 1 2	
1.512E+00	1.453E+02	92	M099	1 2 0 1 2	
1.684E+00	1.618E+02	93	G050	1 0 2 1 2	
4.721E+00	4.536E+02	95.90	E037	1 2 2 2 2	
1.617E+00	1.554E+02	97.90	M099	1 2 0 1 2	

406. $C_5H_4O_2S$

3-Thenoic acid

Thiophen-carbonsaeure-(3)

RN: 88-13-1 **MP** (°C)**:** 137

MW: 128.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.355E-02	4.300E+00	25	F300	1 0 0 0 1	

407. $C_5H_4O_3$
2-Furoic acid
Furan-carbon-saeure-(2)
RN: 88-14-2 **MP** (°C)**:** 129.5
MW: 112.09 **BP** (°C)**:** 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.227E-01	2.496E+01	5.99	A341	0 0 0 0 0	
2.243E-01	2.514E+01	6.99	A341	0 0 0 0 0	
2.332E-01	2.614E+01	10.49	A341	0 0 0 0 0	
2.498E-01	2.799E+01	10.99	A341	0 0 0 0 0	
2.543E-01	2.851E+01	11.99	A341	0 0 0 0 0	
3.310E-01	3.710E+01	15	F300	1 0 0 0 2	
2.606E-01	2.921E+01	15.99	A341	0 0 0 0 0	
3.385E-01	3.794E+01	20.99	A341	0 0 0 0 0	
4.216E-01	4.725E+01	24.99	A341	0 0 0 0 0	
4.665E-01	5.229E+01	27.99	A341	0 0 0 0 0	
5.182E-01	5.808E+01	28.99	A341	0 0 0 0 0	
6.448E-01	7.227E+01	33.99	A341	0 0 0 0 0	
6.677E-01	7.484E+01	35.99	A341	0 0 0 0 0	
7.816E-01	8.761E+01	37.99	A341	0 0 0 0 0	
1.120E+00	1.256E+02	41.99	A341	0 0 0 0 0	
1.229E+00	1.378E+02	43.99	A341	0 0 0 0 0	
1.444E+00	1.618E+02	46.64	A341	0 0 0 0 0	
2.159E+00	2.420E+02	49.99	A341	0 0 0 0 0	
2.610E+00	2.926E+02	51.99	A341	0 0 0 0 0	
2.768E+00	3.103E+02	53.99	A341	0 0 0 0 0	
2.815E+00	3.155E+02	54.49	A341	0 0 0 0 0	
3.221E+00	3.610E+02	54.99	A341	0 0 0 0 0	
3.964E+00	4.443E+02	57.49	A341	0 0 0 0 0	
4.219E+00	4.729E+02	60.04	A341	0 0 0 0 0	
4.224E+00	4.735E+02	61.39	A341	0 0 0 0 0	
4.940E+00	5.537E+02	62.99	A341	0 0 0 0 0	
5.529E+00	6.197E+02	67.99	A341	0 0 0 0 0	
1.838E+00	2.060E+02	100	F300	1 0 0 0 2	

408. $C_5H_4O_3$
Isopyromucic acid
Isobrenzschleimsaeure
RN: 496-64-0 **MP** (°C)**:**
MW: 112.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-01	4.310E+01	0	F300	1 0 0 0 2	

409. $C_5H_5Cl_3N_2OS$
5-Ethoxy-3-trichloromethyl-1,2,4-thiadiazole
RN: 2593-15-9 **MP** (°C)**:**
MW: 247.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.732E-04	1.171E-01	ns	S460	0 0 0 0 0	

410. C_5H_5NO
3-Hydroxypyridine
3-Pyridinol
RN: 109-00-2 **MP** (°C)**:** 127.5
MW: 95.10 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.392E-01	3.226E+01	20	B050	1 0 0 0 0	

411. C_5H_5NO
4-Hydroxypyridine
4-Pyridinol
RN: 626-64-2 **MP** (°C)**:** 148
MW: 95.10 **BP** (°C)**:** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

412. C_5H_5NO
2-Hydroxypyridine
2-Pyridinol
RN: 72762-00-6 **MP** (°C)**:** 106
MW: 95.10 **BP** (°C)**:** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

413. $C_5H_5NO_2$
2,4-Dihydroxypyridine
3-Deazauracil
2,4-Pyridinediol
RN: 626-03-9 **MP** (°C)**:** 278
MW: 111.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.591E-02	6.211E+00	20	B050	1 0 0 0 0	

414. $C_5H_5N_3O$

Pyrazinamide
Pyrazine-2-carboxamide
Prazina

RN: 98-96-4 **MP** (°C)**:** 190
MW: 123.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-01	1.740E+01	25	N041	2 0 1 1 0	EFG
1.218E-01	1.500E+01	ns	K444	0 0 0 0 0	

415. $C_5H_5N_5$

Adenine
Adenin
6-Aminopurine
1H-Purin-6-amine
Adeninimine
Vitamin B4

RN: 73-24-5 **MP** (°C)**:** 363
MW: 135.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E-03	6.377E-01	17.5	S306	1 0 1 2 2	
6.328E-03	8.551E-01	18.8	S306	1 0 1 2 2	
6.494E-03	8.776E-01	19.2	S306	1 0 1 2 2	
7.382E-03	9.975E-01	19.7	S306	1 0 1 2 2	
7.000E-03	9.459E-01	20	C017	2 0 0 1 0	EFG
6.907E-03	9.333E-01	20.08	D307	0 0 0 0 0	
7.680E-03	1.038E+00	22.36	D307	0 0 0 0 0	
6.586E-03	8.900E-01	25	A337	0 0 0 0 0	
7.200E-03	9.729E-01	25	C416	2 1 1 1 1	
5.476E-03	7.400E-01	25	C437	0 0 0 0 0	Average
6.654E-03	8.992E-01	25	D041	1 0 0 0 0	
7.040E-03	9.513E-01	25	H061	0 0 0 0 0	
7.600E-03	1.027E+00	25	L080	2 1 2 1 2	
8.000E-03	1.081E+00	25	R039	0 0 0 0 0	
8.610E-03	1.163E+00	25.01	D307	0 0 0 0 0	
8.690E-03	1.174E+00	25.03	D307	0 0 0 0 0	
8.250E-03	1.115E+00	25.5	T008	1 1 2 2 2	
7.936E-03	1.072E+00	26.6	S306	1 0 1 2 2	
9.740E-03	1.316E+00	27.47	D307	0 0 0 0 0	
1.087E-02	1.469E+00	29.97	D307	0 0 0 0 0	
9.377E-03	1.267E+00	31.1	S306	1 0 1 2 2	
1.540E-02	2.081E+00	37	L042	2 0 2 2 2	pH 6.47
1.390E-02	1.878E+00	38	T008	1 1 2 2 2	
1.514E-02	2.045E+00	44.0	S306	1 0 1 2 2	
1.707E-02	2.307E+00	45.1	S306	1 0 1 2 2	
1.862E-02	2.516E+00	45.5	S306	1 0 1 2 2	

(*continued*)

415. $C_5H_5N_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-01	2.439E+01	100	D041	1 0 0 0 0	
6.808E-03	9.200E-01	c	D004	0 0 0 0 0	
1.805E-01	2.439E+01	h	D004	0 0 0 0 0	

416. $C_5H_5N_5O$

Guanine
2-Aminohypoxanthine
2-Amino-6-hydroxypurine

RN: 73-40-5 **MP** (°C)**:** >300
MW: 151.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	2.902E-03	15.02	D307	0 0 0 0 0	
6.000E-05	9.068E-03	20	C017	2 0 0 1 1	EFG
2.740E-05	4.141E-03	20.05	D307	0 0 0 0 0	
3.290E-05	4.972E-03	22.50	D307	0 0 0 0 0	
3.870E-05	5.849E-03	25.02	D307	0 0 0 0 0	
4.520E-05	6.831E-03	27.54	D307	0 0 0 0 0	
5.350E-05	8.085E-03	30.01	D307	0 0 0 0 0	
7.230E-05	1.093E-02	35.05	D307	0 0 0 0 0	
2.647E-04	4.000E-02	40	D041	1 0 0 0 0	
9.880E-05	1.493E-02	40.22	D307	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R424	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R427	0 0 0 0 0	

417. $C_5H_5N_5O$

Isoguanine
2-Hydroxy-6-aminopurine

RN: 3373-53-3 **MP** (°C)**:**
MW: 151.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.970E-04	6.000E-02	25	D041	1 0 0 0 0	
1.654E-03	2.499E-01	100	D041	1 0 0 0 1	

418. $C_5H_5N_5O_2$

2,8-Dioxyadenine
2,8-Dihydroxyadenine

RN: 30377-37-8 **MP** (°C)**:**
MW: 167.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-05	2.200E-03	25	B049	1 0 1 1 1	
8.556E-06	1.430E-03	37	P068	0 0 0 0 0	

419. C_5H_6

Cyclopentadiene
Pentolex
Pentole
Pyropentylene
R-Pentine
1,3-Cyclopentadiene

RN: 542-92-7 **MP** (°C)**:** –85
MW: 66.10 **BP** (°C)**:** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-02	6.764E-01	ns	S460	0 0 0 0 0	

420. $C_5H_6Cl_2N_2$

3-Methyluracil
2,4(1H,3H)-Pyrimidinedione, 3-methyl-
Uracil, 3-methyl-

RN: 608-34-4 **MP** (°C)**:**
MW: 165.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	2.000E+02	ns	B177	0 0 0 0 2	

421. $C_5H_6Cl_2N_2O_2$

Dantoin
1,3-Dichloro-5,5-dimethyl-2,4-imidazolidinedione
1,3-Dichloro-5,5-dimethylhydantoin

RN: 118-52-5 **MP** (°C)**:** 132
MW: 197.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.537E-03	4.998E-01	20	B080	1 0 1 1 0	
6.590E-03	1.298E+00	40	B080	1 0 1 1 1	

422. $C_5H_6N_2OS$

Methylthiouracil
6-Methyl-2-thiouracil

RN: 56-04-2 **MP** (°C)**:** 330
MW: 142.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-03	5.332E-01	25	G016	1 2 1 2 2	intrinsic
7.026E-03	9.990E-01	c	I310	0 0 0 0 0	
3.715E-03	5.283E-01	ns	R424	0 0 0 0 0	

423. $C_5H_6N_2OS$

5-Methyl-2-thiouracil
4(1H)-Pyrimidinone, 2,3-dihydro-5-methyl-2-thioxo-
2-Thiothymine
RN: 636-26-0 **MP** (°C)**:** 284
MW: 142.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.580E-03	5.090E-01	25	G016	1 2 1 2 2	intrinsic

424. $C_5H_6N_2O_2$

Thymine
2,4-Dihydroxy-5-methylpyrimidine
5-Methyluracil
RN: 65-71-4 **MP** (°C)**:** 316
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	2.775E+00	20	C017	2 0 0 1 1	EFG
2.379E-02	3.000E+00	23	F300	1 0 0 0 0	
3.552E-02	4.480E+00	25	D041	1 0 0 0 1	
2.780E-02	3.506E+00	25	H061	0 0 0 0 0	
3.030E-02	3.821E+00	25	L080	2 1 2 1 2	
2.860E-02	3.607E+00	25	R039	0 0 0 0 0	
2.740E-02	3.456E+00	25.5	T008	1 1 2 2 2	
3.500E-02	4.414E+00	30	L080	2 1 2 1 2	

425. $C_5H_6N_2O_2$

1-Methyluracil
2,4(1H,3H)-Pyrimidinedione, 1-methyl-
*N*1-Methyluracil
RN: 615-77-0 **MP** (°C)**:** 179
MW: 126.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.586E-01	2.000E+01	ns	B177	0 0 0 0 1	

426. $C_5H_6N_2O_4$

5-Carboxymethylhydantoin
Hydantoin of aspartic acid
RN: 5427-26-9 **MP** (°C)**:** 216
MW: 158.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-02	1.115E+01	ns	M025	0 2 0 1 2	

427. $C_5H_6O_2$
α-Angelica lactone
α-Angelica-lacton
RN: 591-12-8 **MP** (°C)**:** 18
MW: 98.10 **BP** (°C)**:** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-01	4.600E+01	15	F300	1 0 0 0 1	

428. $C_5H_6O_4$
Citraconic acid
Citraconsaeure
RN: 498-23-7 **MP** (°C)**:**
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.018E+00	7.830E+02	25	F300	1 0 0 0 2	

429. $C_5H_6O_4$
Mesaconic acid
Mesaconsaeure
RN: 498-24-8 **MP** (°C)**:** 204.5
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.022E-01	2.630E+01	18	F300	1 0 0 0 2	
4.241E+00	5.518E+02	100	F300	1 0 0 0 2	

430. $C_5H_6O_4$
Itaconic acid
Itaconsaeure
RN: 97-65-4 **MP** (°C)**:** 163
MW: 130.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.281E-01	5.570E+01	10	F300	1 0 0 0 2	
5.891E-01	7.664E+01	20	D041	1 0 0 0 1	
5.903E-01	7.680E+01	20	F300	1 0 0 0 2	

431. C_5H_6S

3-Methylthiophene

RN: 616-44-4 **MP** (°C)**:** –69
MW: 98.17 **BP** (°C)**:** 114 at 738 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-03	3.999E-01	ns	S460	0 0 0 0 0	

432. $C_5H_7NO_2$

Ethyl cyanoacetate
Cyanessigsaeure-aethyl ester

RN: 105-56-6 **MP** (°C)**:**
MW: 113.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.768E-01	2.000E+01	25	F300	1 0 0 0 0	
7.072E-01	8.000E+01	80	F300	1 0 0 0 0	

433. $C_5H_7NO_4S$

2,4-Thiazolidinedicarboxylic acid
Tidiacic acid
Tidiacic
TDCA

RN: 30097-06-4 **MP** (°C)**:**
MW: 177.18 **BP** (°C)**:** 524.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-02	7.619E+00	21	B414	1 0 0 1 1	

434. $C_5H_7N_2O_2$

6-Methyluracil
4-Methyl-uracil

RN: 626-48-2 **MP** (°C)**:** 318dec
MW: 127.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.506E-02	7.000E+00	22	F300	1 0 0 0 0	

435. $C_5H_7N_3O$

5-Methylcytosine
Mec

RN: 554-01-8 **MP** (°C)**:** 270
MW: 125.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.441E-01	4.306E+01	25	D041	1 0 0 0 1	

436. $C_5H_7N_3O_2$
Dimetridazole
1,2-Dimethyl-5-nitroimidazole
RN: 551-92-8 **MP** (°C)**:** 137–139
MW: 141.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.738E-02	9.509E+00	20	D344	0 0 0 0 0	
6.870E-02	9.696E+00	20	D344	0 0 0 0 0	

437. C_5H_8
Isoprene
2-Methyl-1,3-butadiene
RN: 78-79-5 **MP** (°C)**:** –120
MW: 68.12 **BP** (°C)**:** 34.07

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.425E-03	6.420E-01	25	M001	2 1 2 2 2	

438. C_5H_8
Cyclopentene
RN: 142-29-0 **MP** (°C)**:** –135
MW: 68.12 **BP** (°C)**:** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.411E-02	1.642E+00	24.8	L007	2 1 1 2 2	
7.854E-03	5.350E-01	25	M001	2 1 2 2 2	
2.411E-02	1.642E+00	25.1	L007	2 2 1 1 2	
2.562E-02	1.745E+00	34.8	L007	2 1 1 2 2	

439. C_5H_8
1-Pentyne
Pent-1-yne
RN: 627-19-0 **MP** (°C)**:** –106
MW: 68.12 **BP** (°C)**:** 40

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.305E-02	1.570E+00	25	M001	2 1 2 2 2	
1.154E-02	7.861E-01	25	M342	1 0 1 1 2	

440. C_5H_8
1,4-Pentadiene
Penta-1,4-diene
RN: 591-93-5 **MP** (°C)**:** –148
MW: 68.12 **BP** (°C)**:** 26

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.191E-03	5.580E-01	25	M001	2 1 2 2 2	

441. $C_5H_8BrNO_4$
5-Bromo-2-methyl-5-nitro-1,3-dioxane
Dioxane, 5-bromo-2-methyl-5-nitro-
Nibroxane
RN: 53983-00-9 **MP** (°C)**:** 72
MW: 226.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.695E-02	6.093E+00	25	L013	1 0 2 1 2	

442. $C_5H_8N_2O_2$
5,5′-Dimethylhydantoin
5,5-Dimethylhydantoin
5,5-Dimethyl-2,4-imidazolidinedione
5,5-Dimethylimidazolidine-2,4-dione
RN: 77-71-4 **MP** (°C)**:** 177
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.304E+02	37	F183	1 0 1 1 1	intrinsic

443. $C_5H_8N_2O_2$
5-Ethylhydantoin
Hydantoin of α-aminobutyric acid
RN: 15414-82-1 **MP** (°C)**:** 119
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-01	1.106E+02	ns	M025	0 2 0 1 2	

444. $C_5H_8N_4O_3S_2$

Methazolamide
Acetamide, *N*-[5-(aminosulfonyl)-3-methyl-1,3,4-thiadiazol-2(3H)-ylidene]-
N-(4-Methyl-2-sulfamoyl-D2-1,3,4-thiadiazolin-5-ylidene)acetamide
Neptazaneat
Metazolamide
Methenamide

RN: 554-57-4 **MP** (°C)**:** 213
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.725E-01	15	K024	1 2 1 1 1	
1.200E-02	2.835E+00	25	C415	1 0 0 1 0	
2.963E-03	7.000E-01	amb	L434	0 0 0 0 0	
1.481E-02	3.500E+00	ns	M032	0 0 0 0 2	
1.479E-02	3.495E+00	ns	R428	0 0 0 0 0	

445. $C_5H_8N_4O_{12}$

Pentaerythritol tetranitrate
Nitropentaerythritol
1,3-Propanediol, 2,2-*bis*[(nitrooxy)methyl]-, dinitrate (ester)

RN: 78-11-5 **MP** (°C)**:** 140
MW: 316.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.326E-06	2.000E-03	ns	M013	0 2 0 1 1	

446. C_5H_8O

Cyprethylene ether

RN: **MP** (°C)**:**
MW: 84.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.435E-02	7.937E+00	27	K058	1 0 1 1 0	

447. C_5H_8O

α-Methylcrotonaldehyde
α-Methyl-crotonaldehyd

RN: 623-36-9 **MP** (°C)**:**
MW: 84.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	2.000E+01	20	F300	1 0 0 0 1	

448. $C_5H_8O_2$
Ethyl acrylate
Ethyl propenoate
2-Propenoic acid ethyl ester
RN: 140-88-5 **MP** (°C)**:** –71
MW: 100.12 **BP** (°C)**:** 99.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.785E-01	1.787E+01	30	L096	1 2 0 2 2	

449. $C_5H_8O_2$
Methyl methacrylate
Methacrylic acid methyl ester
Methyl 2-methyl-2-propenoate
RN: 80-62-6 **MP** (°C)**:** –48
MW: 100.12 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.563E-01	1.565E+01	20	L096	1 2 0 2 2	

450. $C_5H_8O_2$
Acetylacetone
2,4-Pentanedione
Acetylaceton
RN: 123-54-6 **MP** (°C)**:** –23
MW: 100.12 **BP** (°C)**:** 140.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E+00	1.680E+02	19.0	N051	1 2 1 1 2	
1.703E+00	1.705E+02	19.5	N051	1 2 1 1 2	
1.089E+00	1.090E+02	20	F300	1 0 0 0 2	
1.706E+00	1.708E+02	25	B019	1 0 1 2 0	

451. $C_5H_8O_3$
Dimethylpyruvic acid
DL-Methyl-bernsteinsaeure
α-Ketoisovaleric acid
RN: 759-05-7 **MP** (°C)**:**
MW: 116.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E+00	4.006E+02	20	F300	1 0 0 0 2	

452. $C_5H_8O_3$
Levulinic acid
Laevulinsaeure
4-Oxopentanoic acid
3-Acetyl propionic acid
RN: 123-76-2 **MP** (°C)**:** 37.2
MW: 116.12 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.632E+00	5.378E+02	6.99	A340	0 0 0 0 0	
4.990E+00	5.795E+02	9.99	A340	0 0 0 0 0	
5.530E+00	6.422E+02	14.49	A340	0 0 0 0 0	
6.087E+00	7.068E+02	20.79	A340	0 0 0 0 0	
6.400E+00	7.431E+02	24.99	A340	0 0 0 0 0	
6.631E+00	7.700E+02	30.09	A340	0 0 0 0 0	

453. $C_5H_8O_4$
Methylsuccinic acid
Acide methylsuccinique
1,2-Propanedicarboxylic acid
RN: 498-21-5 **MP** (°C)**:** 117.5
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E+00	6.660E+02	15	M051	1 0 0 0 2	

454. $C_5H_8O_4$
Ethylmalonic acid
1,1-Propanedicarboxylic acid
Aethylmalonsaeure
Mono-ethyl malonate
Malonic acid monoethyl ester
Malonsaeure-monoaethyl ester
RN: 601-75-2 **MP** (°C)**:** 114
MW: 132.12 **BP** (°C)**:** 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E+00	3.460E+02	0	F300	1 0 0 0 2	
3.996E+00	5.280E+02	0	M051	1 0 0 0 2	
4.814E+00	6.360E+02	15	M051	1 0 0 0 2	
5.389E+00	7.120E+02	25	M051	1 0 0 0 2	
3.626E+00	4.790E+02	50	F300	1 0 0 0 2	
6.873E+00	9.080E+02	50	M051	1 0 0 0 2	

455. $C_5H_8O_4$
Dimethylmalonic acid
Dimethyl-malonsaeure
Dimethyl-propanedioic acid
RN: 595-46-0 **MP** (°C)**:** 192
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.812E-01	9.000E+01	13	F300	1 0 0 0 0	
1.968E+00	2.600E+02	100	F300	1 0 0 0 1	

456. $C_5H_8O_4$
Glutaric acid
Glutarsaeure
1,3-Propanedicarboxylic acid
RN: 110-94-1 **MP** (°C)**:** 96.5
MW: 132.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.272E+00	3.002E+02	0	F300	1 0 0 0 2	
3.247E+00	4.290E+02	0	L041	1 0 0 1 2	
2.410E+00	3.183E+02	3.40	A031	1 2 2 2 2	
2.650E+00	3.501E+02	5.99	A341	0 0 0 0 0	
2.764E+00	3.651E+02	7.99	A341	0 0 0 0 0	
3.127E+00	4.131E+02	10.40	A031	1 2 2 2 2	
2.909E+00	3.843E+02	10.99	A341	0 0 0 0 0	
3.213E+00	4.245E+02	12.99	A341	0 0 0 0 0	
3.433E+00	4.536E+02	14	A031	1 2 2 2 0	
4.443E+00	5.870E+02	15	L041	1 0 0 1 2	
4.443E+00	5.870E+02	15	M051	1 0 0 0 2	
3.521E+00	4.652E+02	15.99	A341	0 0 0 0 0	
3.674E+00	4.854E+02	17.99	A341	0 0 0 0 0	
3.861E+00	5.100E+02	18	A031	1 2 2 2 2	
3.816E+00	5.041E+02	19.99	A341	0 0 0 0 0	
2.954E+00	3.902E+02	20	D041	1 0 0 0 1	
4.837E+00	6.390E+02	20	L041	1 0 0 1 2	
2.952E+00	3.900E+02	20	M171	1 0 0 0 2	
1.340E+00	1.770E+02	20	S006	1 0 0 0 2	
4.278E+00	5.652E+02	23.90	A031	1 2 2 2 2	
4.088E+00	5.401E+02	24.99	A341	0 0 0 0 0	
4.653E+00	6.148E+02	28.30	A031	1 2 2 2 2	
4.394E+00	5.805E+02	28.99	A341	0 0 0 0 0	
4.503E+00	5.949E+02	30.99	A341	0 0 0 0 0	
4.642E+00	6.133E+02	33.99	A341	0 0 0 0 0	
6.033E+00	7.970E+02	35	L041	1 0 0 1 2	
4.796E+00	6.336E+02	36.99	A341	0 0 0 0 0	
4.894E+00	6.466E+02	38.99	A341	0 0 0 0 0	
5.096E+00	6.732E+02	42.99	A341	0 0 0 0 0	
5.131E+00	6.779E+02	43.99	A341	0 0 0 0 0	
5.143E+00	6.795E+02	44.99	A341	0 0 0 0 0	

(*continued*)

456. $C_5H_8O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.246E+00	6.930E+02	46.99	A341	0 0 0 0 0	
5.341E+00	7.057E+02	49.99	A341	0 0 0 0 0	
7.244E+00	9.570E+02	50	L041	1 0 0 1 2	
5.470E+00	7.227E+02	54.49	A341	0 0 0 0 0	
5.640E+00	7.451E+02	55.99	A341	0 0 0 0 0	
5.713E+00	7.548E+02	58.99	A341	0 0 0 0 0	
5.729E+00	7.569E+02	61.09	A341	0 0 0 0 0	
5.890E+00	7.782E+02	62.99	A341	0 0 0 0 0	
4.032E+00	5.327E+02	65	F300	1 0 0 0 2	
8.462E+00	1.118E+03	65	L041	1 0 0 1 2	
6.038E+00	7.977E+02	68.99	A341	0 0 0 0 0	
4.081E+00	5.392E+02	rt	H431	0 0 0 0 0	

457. $C_5H_9BrO_2$

α-Bromo-methyl-ethyl-acetate
Ethyl DL-α-bromopropionate
Propanoic acid, 2-bromo-, ethyl ester
Ethyl DL-2-bromopropionate

RN: 535-11-5 **MP** (°C)**:**
MW: 181.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-01	5.033E+01	ns	F057	0 2 2 2 1	

458. $C_5H_9BrO_2$

α-Ethyl-β-bromo-propionic ureide

RN: **MP** (°C)**:**
MW: 181.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-01	3.855E+01	ns	F056	0 2 2 2 1	

459. $C_5H_9NO_2$

DL-Proline
Pyrrolidine-2-carboxylic acid

RN: 609-36-9 **MP** (°C)**:** 208
MW: 115.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.217E+01	1.401E+03	20	J303	0 0 0 0 0	
1.146E+01	1.319E+03	25	J303	0 0 0 0 0	
1.425E+01	1.641E+03	40	J303	0 0 0 0 0	
1.708E+01	1.967E+03	50	J303	0 0 0 0 0	
2.082E+01	2.397E+03	60	J303	0 0 0 0 0	

460. $C_5H_9NO_2$
L-Proline
2-Pyrrolidinecarboxylic acid
RN: 147-85-3 **MP** (°C)**:**
MW: 115.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E+00	6.188E+02	25	D041	1 0 0 0 2	
6.653E+00	7.660E+02	27	D036	0 0 0 0 0	
6.123E+00	7.050E+02	65	D041	1 0 0 0 2	
6.691E+00	7.704E+02	99.99	P349	0 0 0 0 0	

461. $C_5H_9NO_2S$
2-Methylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-methyl-
Thiazolidine-4-carboxylic acid, 2-methyl-
RN: 4165-32-6 **MP** (°C)**:** 174-175
MW: 147.20 **BP** (°C)**:** 333.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-01	3.091E+01	21	B414	1 0 0 1 1	partial decomposition

462. $C_5H_9NO_3$
L-Hydroxyproline
trans-4-Hydroxy-L-proline
L-4-hydroxyproline
(4*S*)-4-Hydroxy-L-proline
RN: 51-35-4 **MP** (°C)**:**
MW: 131.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.158E+00	4.141E+02	99.99	P349	0 0 0 0 0	

463. $C_5H_9NO_3$
Formyl-α-aminobutyric acid
Butanoic acid, 2-(formylamino)-
RN: 106873-99-8 **MP** (°C)**:**
MW: 131.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-01	3.357E+01	25	M024	1 2 0 1 2	
2.560E-01	3.357E+01	ns	M025	0 2 0 1 2	

464. $C_5H_9NO_4$

D-Glutamic acid
D-2-Aminoglutaric acid
RN: 6893-26-1 **MP** (°C)**:** 201
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-02	3.439E+00	0	D018	2 2 2 1 2	
2.303E-02	3.388E+00	0	M043	1 0 0 0 1	
3.381E-02	4.975E+00	10	M043	1 0 0 0 1	
1.004E-01	1.478E+01	20	D041	1 0 0 0 1	
4.859E-02	7.149E+00	20	M043	1 0 0 0 1	
4.472E-02	6.580E+00	21	P045	1 0 2 1 2	
5.981E-02	8.800E+00	25	D018	2 2 2 1 2	
6.729E-02	9.901E+00	30	M043	1 0 0 0 1	
1.004E-01	1.478E+01	40	M043	1 0 0 0 1	
1.481E-01	2.179E+01	50	D018	2 2 2 1 2	
2.107E-01	3.101E+01	60	M043	1 0 0 0 1	
4.148E-01	6.103E+01	80	M043	1 0 0 0 1	
8.347E-01	1.228E+02	100	M043	1 0 0 0 2	
5.850E-02	8.607E+00	ns	M025	0 2 0 1 2	

465. $C_5H_9NO_4$

DL-Glutamic acid
DL-2-Aminoglutaric acid
RN: 617-65-2 **MP** (°C)**:** 194
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-02	8.241E+00	0	D018	2 2 2 1 2	
4.850E-02	7.136E+00	4.99	A405	2 0 1 1 2	
5.990E-02	8.813E+00	9.99	A405	2 0 1 1 2	
6.300E-02	9.269E+00	14.99	A405	2 0 1 1 2	
8.840E-02	1.301E+01	20.99	A405	2 0 1 1 2	
9.370E-02	1.379E+01	24.99	A405	2 0 1 1 2	
1.750E-01	2.575E+01	25	D018	2 2 2 1 2	
1.368E-01	2.013E+01	25	D041	1 0 0 0 2	
1.075E-01	1.582E+01	29.99	A405	2 0 1 1 2	
1.414E-01	2.080E+01	34.99	A405	2 0 1 1 2	
1.684E-01	2.478E+01	39.99	A405	2 0 1 1 2	
2.016E-01	2.966E+01	44.99	A405	2 0 1 1 2	
2.699E-01	3.971E+01	49.99	A405	2 0 1 1 2	
5.131E-01	7.549E+01	50	D018	2 2 2 1 2	
3.502E-01	5.153E+01	54.99	A405	2 0 1 1 2	
3.959E-01	5.825E+01	59.99	A405	2 0 1 1 2	
4.772E-01	7.021E+01	64.99	A405	2 0 1 1 2	
5.621E-01	8.270E+01	69.99	A405	2 0 1 1 2	
6.709E-01	9.871E+01	71.99	A405	2 0 1 1 2	
7.289E-01	1.072E+02	74.99	A405	2 0 1 1 2	
7.206E-01	1.060E+02	75	D041	1 0 0 0 2	

466. $C_5H_9NO_4$
L-Glutamic acid
L-2-Aminoglutaric acid
L(+)-Glutaminsaeure
Glutamic acid
L(+) Glutaminic acid
RN: 56-86-0 **MP** (°C)**:** 250
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.866E-02	7.160E+00	20	B032	1 2 2 1 2	
4.486E-02	6.600E+00	21	F302	1 0 0 0 1	
5.825E-02	8.570E+00	25	B032	1 2 2 1 2	
5.822E-02	8.566E+00	25	D041	1 0 0 0 2	
5.845E-02	8.600E+00	25	F300	1 0 0 0 1	
7.262E-02	1.068E+01	25	G315	0 0 0 0 0	
5.614E-02	8.260E+00	27	D036	0 0 0 0 0	
6.980E-02	1.027E+01	29.80	B032	1 2 2 1 2	
1.454E-01	2.140E+01	50	F300	1 0 0 0 2	
3.562E-01	5.240E+01	75	D041	1 0 0 0 2	
3.561E-01	5.240E+01	75	F300	1 0 0 0 2	
8.346E-01	1.228E+02	100	F300	1 0 0 0 2	
4.078E-02	6.000E+00	ns	D072	0 0 0 0 0	
5.802E-02	8.537E+00	rt	H431	0 0 0 0 0	

467. C_5H_{10}
Cyclopentane
Pentamethylene
Exxsol cyclopentane S
Zeonsolv HP
RN: 287-92-3 **MP** (°C)**:** –94.4
MW: 70.14 **BP** (°C)**:** 49.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.826E-03	3.385E-01	4.8	L007	2 2 1 2 2	
4.826E-03	3.385E-01	5.1	L007	2 1 1 1 2	
4.870E-03	3.416E-01	14.8	L007	2 2 1 2 2	
4.870E-03	3.416E-01	15.2	L007	2 1 1 1 2	
4.873E-03	3.418E-01	24.8	L007	2 2 1 2 2	
2.338E-03	1.640E-01	25	G313	2 1 1 2 2	
2.281E-03	1.600E-01	25	K119	1 0 0 0 2	
2.224E-03	1.560E-01	25	M001	2 1 2 2 2	
2.224E-03	1.560E-01	25	M002	2 1 2 2 2	
2.281E-03	1.600E-01	25.0	P051	2 1 1 2 2	
2.281E-03	1.600E-01	25.00	P007	2 1 2 2 2	
4.873E-03	3.418E-01	25.1	L007	2 1 1 1 2	
5.252E-03	3.684E-01	34.8	L007	2 2 1 2 2	
5.252E-03	3.684E-01	35.2	L007	2 1 1 1 2	
2.324E-03	1.630E-01	40.1	P051	2 1 1 2 2	

(*continued*)

467. C_5H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-03	1.630E-01	40.10	P007	2 1 2 2 2	
4.867E-03	3.414E-01	44.8	L007	2 2 1 2 2	
2.566E-03	1.800E-01	55.7	P051	2 1 1 2 2	
2.566E-03	1.800E-01	55.70	P007	2 1 2 2 2	
4.220E-03	2.960E-01	99.1	P051	2 1 1 2 2	
4.220E-03	2.960E-01	99.10	P007	2 1 2 2 2	
5.304E-03	3.720E-01	118.0	P051	2 1 1 2 2	
5.304E-03	3.720E-01	118.00	P007	2 1 2 2 2	
8.712E-03	6.110E-01	137.3	P051	2 1 1 2 2	
8.712E-03	6.110E-01	137.30	P007	2 1 2 2 2	
1.129E-02	7.920E-01	153.1	P051	2 1 1 2 2	
1.129E-02	7.920E-01	153.10	P007	2 1 2 2 2	
2.224E-03	1.560E-01	ns	H123	0 0 0 0 0	

468. C_5H_{10}

3-Methyl-1-butene
2-Methyl-3-butene
3,3-Dimethylpropene
Isopropylethylene

RN: 563-45-1 **MP** (°C)**:** –168
MW: 70.14 **BP** (°C)**:** 20

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-03	1.300E-01	25	M001	2 1 2 2 2	

469. C_5H_{10}

2-Pentene
1-Methyl-2-ethylethylene
sym-Methylethylethylene
β-Amylene
β-*n*-Amylene
3-Pentene

RN: 109-68-2 **MP** (°C)**:** –136
MW: 70.14 **BP** (°C)**:** 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-03	2.030E-01	25	M001	2 1 2 2 2	

470. C_5H_{10}
1-Pentene
Propylethylene
α-*n*-Amylene
1-Methyl-3-butene
RN: 109-67-1 **MP** (°C)**:** –165
MW: 70.14 **BP** (°C)**:** 30.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-03	1.830E-01	23	C332	0 0 0 0 0	
2.110E-03	1.480E-01	25	M001	2 1 2 2 2	

471. $C_5H_{10}Cl_3O_3P$
Diethyl trichloromethyl phosphonate
Phosphonic acid, (trichloromethyl)-, diethyl ester
Ro 3-0658
RN: 866-23-9 **MP** (°C)**:**
MW: 255.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-02	4.500E+00	25	B070	1 2 0 1 1	

472. $C_5H_{10}N_2O$
N-Nitrosopiperidine
Pyridine, hexahydro-*N*-nitroso
NPIP
RN: 100-75-4 **MP** (°C)**:** <25
MW: 114.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	7.648E+01	24	D083	2 0 0 0 1	

473. $C_5H_{10}N_2O_2S$
Methomyl
Nudrin
Lannate
RN: 16752-77-5 **MP** (°C)**:** 78.5
MW: 162.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-01	5.800E+01	25	M161	1 0 0 0 1	

474. $C_5H_{10}N_2O_3$
Glycolylglycineamide
RN: **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E+00	8.506E+02	25	M008	1 0 0 0 2	

475. $C_5H_{10}N_2O_3$
Glycyl-L-alanine
Glycylalanine
RN: 3695-73-6 **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E+00	6.986E+02	24.99	B441	0 0 0 0 0	

476. $C_5H_{10}N_2O_3$
D-Glutamine
D-2-Aminoglutaramic acid
RN: 5959-95-5 **MP** (°C)**:**
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.910E-01	4.253E+01	ns	M025	0 2 0 1 2	

477. $C_5H_{10}N_2O_3$
L-Glutamine
L(+)-Glutamin
L(+)-Glutamine
Glutamine
RN: 56-85-9 **MP** (°C)**:** 185
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.184E-01	1.730E+01	0	F300	1 0 0 0 2	
2.378E-01	3.475E+01	18	D041	1 0 0 0 1	
2.444E-01	3.572E+01	20	B032	1 2 2 1 2	
2.829E-01	4.135E+01	25	B032	1 2 2 1 2	
2.789E-01	4.077E+01	25	D041	1 0 0 0 2	
2.701E-01	3.948E+01	25	G315	0 0 0 0 0	
5.891E-02	8.610E+00	25	J303	0 0 0 0 0	
2.997E-01	4.380E+01	25.1	N024	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N025	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N026	0 0 0 0 0	

(*continued*)

477. $C_5H_{10}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.821E-01	4.123E+01	25.1	N027	1 1 2 2 2	
2.737E-01	4.000E+01	27	D036	0 0 0 0 0	
3.285E-01	4.801E+01	29.80	B032	1 2 2 1 2	
3.154E-01	4.610E+01	30	F300	1 0 0 0 2	
1.002E-01	1.464E+01	40	J303	0 0 0 0 0	
2.135E-01	3.120E+01	60	J303	0 0 0 0 0	

478. $C_5H_{10}N_2S_2$

Dazomet
3,5-Dimethyl-1,2,3,5-tetrahydro-1,3,5-thiadiazinethione-2
Thiazone
Thiazon

RN: 533-74-4 **MP** (°C)**:** 106.5
MW: 162.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.386E-03	1.199E+00	25	M061	1 0 0 0 1	
1.169E-02	1.896E+00	30	B185	0 0 0 0 0	
7.395E-03	1.200E+00	30	M161	1 0 0 0 1	

479. $C_5H_{10}N_6O_2$

Dinitrosopentamethylenetetramine
3,7-Dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane

RN: 101-25-7 **MP** (°C)**:** 207
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.318E-02	9.901E+00	ns	I313	0 0 0 0 0	

480. $C_5H_{10}O$

Methy propyl ketone
Methyl propyl ketone
2-Pentanone
Pentan-2-one

RN: 107-87-9 **MP** (°C)**:** –78
MW: 86.13 **BP** (°C)**:** 100.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.870E-01	7.640E+01	10	G032	1 2 1 1 2	
6.520E-01	5.616E+01	20	G030	1 2 0 0 2	
5.000E-01	4.307E+01	20	M312	1 0 0 0 1	
6.799E-01	5.857E+01	25	A356	0 0 0 0 0	
4.786E-01	4.123E+01	25	B060	2 0 1 1 1	

(*continued*)

480. $C_5H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-01	6.697E+01	25	C333	0 0 0 0 0	
7.000E-01	6.029E+01	25	F044	1 0 0 0 1	
6.063E-01	5.222E+01	25	G030	1 2 0 0 2	
6.572E-01	5.660E+01	25	P055	1 0 0 0 2	
5.718E-01	4.925E+01	30	G030	1 2 0 0 2	
6.300E-01	5.426E+01	30	G032	1 2 1 1 2	
5.806E-01	5.001E+01	35	A356	0 0 0 0 0	
6.799E-01	5.857E+01	35	C333	0 0 0 0 0	
5.302E-01	4.567E+01	45	A356	0 0 0 0 0	
6.799E-01	5.857E+01	45	C333	0 0 0 0 0	
5.150E-01	4.436E+01	50	G032	1 2 1 1 2	
5.302E-01	4.567E+01	55	A356	0 0 0 0 0	
5.806E-01	5.001E+01	55	C333	0 0 0 0 0	

481. $C_5H_{10}O$

Valeraldehyde
n-Valeraldehyde
Valeral
n-Pentanal

RN: 110-62-3 **MP** (°C)**:** –92
MW: 86.13 **BP** (°C)**:** 103

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-01	1.170E+01	25	A049	1 0 0 0 2	
2.100E-01	1.809E+01	25	K012	1 0 0 0 1	

482. $C_5H_{10}O$

Tetrahydropyran
Pentamethylene oxide

RN: 142-68-7 **MP** (°C)**:** –49.2
MW: 86.13 **BP** (°C)**:** 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.372E+00	1.182E+02	0	B001	2 0 1 0 0	
1.122E+00	9.666E+01	10	B001	2 0 1 0 0	
1.021E+00	8.792E+01	15	B001	2 0 1 0 0	
9.351E-01	8.054E+01	20	B001	2 0 1 0 0	
8.620E-01	7.425E+01	25	B001	2 0 1 0 0	

483. $C_5H_{10}O$
Diethyl ketone
3-Pentanone
RN: 96-22-0 **MP** (°C)**:** –42
MW: 86.13 **BP** (°C)**:** 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-01	6.727E+01	10	G032	1 2 1 1 2	
4.786E-01	4.123E+01	20	D052	1 1 0 0 1	
5.613E-01	4.834E+01	20	G030	1 2 0 0 2	
6.052E-01	5.213E+01	25	B019	1 0 1 2 0	
3.818E-01	3.288E+01	25	B060	2 0 1 1 1	
5.328E-01	4.589E+01	25	G030	1 2 0 0 2	
5.900E-01	5.082E+01	25	K012	1 0 0 0 1	
4.999E-01	4.306E+01	30	G030	1 2 0 0 1	
5.760E-01	4.961E+01	30	G032	1 2 1 1 2	
4.560E-01	3.928E+01	50	G032	1 2 1 1 2	

484. $C_5H_{10}O$
1-Penten-3-ol
Penten-1-ol-3
RN: 616-25-1 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.312E-01	8.021E+01	20	G031	1 0 0 0 2	
8.798E-01	7.579E+01	25	G031	1 0 0 0 2	
8.340E-01	7.184E+01	30	G031	1 0 0 0 2	

485. $C_5H_{10}O$
4-Penten-1-ol
Penten-4-ol-1
RN: 821-09-0 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 135.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.458E-01	5.562E+01	20	G031	1 0 0 0 2	
6.261E-01	5.393E+01	25	G031	1 0 0 0 2	
6.115E-01	5.267E+01	30	G031	1 0 0 0 2	

486. $C_5H_{10}O$
3-Penten-2-ol
Penten-3-ol-2
RN: 1569-50-2 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	8.642E+01	20	G031	1 0 0 0 2	
9.508E-01	8.189E+01	25	G031	1 0 0 0 2	
9.075E-01	7.817E+01	30	G031	1 0 0 0 2	

487. $C_5H_{10}O$
2-Methyl tetrahydrofuran
2-Methyl oxolane
β-Methyl tetramethylene oxide
RN: 96-47-9 **MP** (°C)**:** –136
MW: 86.13 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E+00	1.011E+02	10	B001	2 0 1 0 0	

488. $C_5H_{10}O$
1-Methyl tetrahydrofuran
Methyl oxolane
α-Methyl tetramethylene oxide
RN: 45376-90-7 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.101E+00	1.810E+02	0	B001	2 0 1 0 0	
1.788E+00	1.540E+02	10	B001	2 0 1 0 0	
1.646E+00	1.418E+02	15	B001	2 0 1 0 0	
1.519E+00	1.308E+02	20	B001	2 0 1 0 0	
1.414E+00	1.218E+02	25	B001	2 0 1 0 0	

489. $C_5H_{10}O$
Cypreth ether
Cyclopropane, ethoxy-
Ethoxycyclopropane
Ethyl cyclopropyl ether
RN: 5614-38-0 **MP** (°C)**:**
MW: 86.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	2.724E+01	25	K061	1 0 1 1 1	
2.500E-01	2.153E+01	25	K061	1 0 1 1 1	

490. $C_5H_{10}O$

3-Methyl-2-butanone
3-Methylbutanone-2

RN: 563-80-4 **MP** (°C)**:** –92
MW: 86.13 **BP** (°C)**:** 94.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.130E-01	7.003E+01	10	G032	1 2 1 1 2	
7.116E-01	6.130E+01	20	G030	1 2 0 0 2	
6.654E-01	5.732E+01	25	G030	1 2 0 0 2	
6.240E-01	5.375E+01	30	G030	1 2 0 0 2	
6.080E-01	5.237E+01	30	G032	1 2 1 1 2	
5.940E-01	5.116E+01	50	G032	1 2 1 1 2	

491. $C_5H_{10}OS_2$

Butylxanthogenic acid

RN: **MP** (°C)**:**
MW: 150.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	1.202E-01	25	K012	1 0 0 0 0	

492. $C_5H_{10}O_2$

Valeric acid
Valeric acid, normal
n-Valeric acid

RN: 109-52-4 **MP** (°C)**:** –34.5
MW: 102.13 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.295E-01	2.344E+01	25	B060	2 0 1 1 1	
4.636E-01	4.735E+01	25	H028	2 0 2 0 2	
3.697E-01	3.776E+01	25	H122	1 0 0 0 2	
4.055E-01	4.141E+01	25	H338	2 2 1 2 2	
3.750E-01	3.830E+01	25	K012	1 0 0 0 2	
4.893E-01	4.997E+01	35	H338	2 2 1 2 2	
2.936E-03	2.999E-01	c	L055	0 0 0 0 1	
4.636E-01	4.735E+01	ns	A406	0 0 0 0 1	

493. $C_5H_{10}O_2$
Methyl butyrate
Buttersaeure-methyl ester
n-Methyl *n*-butyrate
RN: 623-42-7 **MP** (°C)**:** –95
MW: 102.13 **BP** (°C)**:** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-01	1.561E+01	21	F001	1 0 1 2 2	
1.506E-01	1.538E+01	21	F300	1 0 0 0 2	
1.600E-01	1.634E+01	21	S006	1 0 0 0 2	
1.469E-01	1.500E+01	25	A049	1 0 0 0 2	

494. $C_5H_{10}O_2$
3-Hydroxy-2-methyltetrahydrofuran
3-Furanol, tetrahydro-2-methyl-
RN: 29848-44-0 **MP** (°C)**:**
MW: 102.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E+00	1.667E+02	rt	B066	0 2 0 0 1	
4.896E+00	5.000E+02	rt	B066	0 2 0 0 2	

495. $C_5H_{10}O_2$
Propyl acetate
Essigsaeurepropyl ester
RN: 109-60-4 **MP** (°C)**:** –92
MW: 102.13 **BP** (°C)**:** 101.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-01	2.270E+01	20	E002	1 0 0 0 2	
1.850E-01	1.889E+01	20	F001	1 0 1 0 2	
1.821E-01	1.860E+01	20	F300	1 0 0 0 2	
1.800E-01	1.838E+01	20	M171	1 0 0 0 1	
2.220E-01	2.267E+01	21	S006	1 0 0 0 2	
1.920E-01	1.961E+01	25	B060	2 0 1 1 1	
1.731E-01	1.768E+01	30	R318	1 2 0 1 1	
1.960E-01	2.002E+01	37	E028	1 0 1 1 2	

496. $C_5H_{10}O_2$
Pivalic acid
Trimethylacetic acid
Trimethylessigsaeure
RN: 75-98-9 **MP** (°C)**:** 35.5
MW: 102.13 **BP** (°C)**:** 163.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-01	2.170E+01	20	F300	1 0 0 0 2	

497. $C_5H_{10}O_2$
Isopropyl acetate
Essigsaeureisopropyl ester
Iso-propylacetat
RN: 108-21-4 **MP** (°C)**:** –73
MW: 102.13 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-01	2.610E+01	20	D052	1 1 0 0 2	average of 2
3.030E-01	3.095E+01	20	F001	1 0 1 2 2	
2.937E-01	3.000E+01	20	F300	1 0 0 0 2	
2.108E-01	2.153E+01	24.6	H121	2 0 0 0 1	
2.759E-01	2.818E+01	25	B060	2 0 1 1 1	
1.930E-01	1.971E+01	37	E028	1 0 1 1 2	

498. $C_5H_{10}O_2$
Butyl formate
Formic acid butyl ester
RN: 592-84-7 **MP** (°C)**:**
MW: 102.13 **BP** (°C)**:** 106.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-02	1.001E+01	22	S006	1 0 0 0 1	
6.400E-02	6.537E+00	25	K012	1 0 0 0 1	
7.400E-02	7.558E+00	27	B052	1 0 1 1 2	
7.500E-02	7.660E+00	30.5	N014	0 0 0 0 0	
8.100E-02	8.273E+00	40.0	N014	0 0 0 0 0	

499. $C_5H_{10}O_2$
Ethyl propionate
Propanoic acid ethyl ester
RN: 105-37-3 **MP** (°C)**:** –73
MW: 102.13 **BP** (°C)**:** 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.844E-01	1.884E+01	20	D052	1 1 0 0 2	
2.200E-01	2.247E+01	20	S006	1 0 0 0 1	
2.154E-01	2.200E+01	25	F300	1 0 0 0 1	
1.700E-01	1.736E+01	25	K012	1 0 0 0 1	
2.108E-01	2.153E+01	30	R318	1 1 0 1 1	

500. $C_5H_{10}O_2$
Isovaleric acid
Isovaleriansaeure
RN: 503-74-2 **MP** (°C)**:** –29.3
MW: 102.13 **BP** (°C)**:** 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.946E-01	4.031E+01	20	D041	1 0 0 0 1	
3.985E-01	4.070E+01	20	F300	1 0 0 0 2	

501. $C_5H_{10}O_3$
Methyl β-methoxypropionate
Propionic acid, 3-methoxy-, methyl ester
Methyl 3-methoxypropanoate
Methyl 3-methoxypropionate
RN: 3852-09-3 **MP** (°C)**:**
MW: 118.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E+00	4.286E+02	25	R034	1 0 0 0 1	

502. $C_5H_{10}O_3$
Ethyl carbonate
Diethyl carbonate
RN: 105-58-8 **MP** (°C)**:** –43
MW: 118.13 **BP** (°C)**:** 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-01	1.845E+01	20	D052	1 1 0 0 2	

503. $C_5H_{10}O_5$
D-Xylose
α-Xylose
Wood sugar
RN: 58-86-6 **MP** (°C)**:** 144.5
MW: 150.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E+00	4.322E+02	25	G317	0 0 0 0 0	

504. $C_5H_{10}O_5$
L-Arabinose
L-Arabinopyranose
RN: 87-72-9 **MP** (°C)**:** 158
MW: 150.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E+00	3.726E+02	10	F300	1 0 0 0 2	

505. $C_5H_{11}Br$
n-Amyl bromide
1-Bromopentane
Pentyl bromide
Amylene bromide
RN: 110-53-2 **MP** (°C)**:** –87.9
MW: 151.05 **BP** (°C)**:** 129.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.380E-04	1.266E-01	25	M342	1 0 1 1 2	
1.800E-02	2.719E+00	ns	H307	0 0 0 0 0	

506. $C_5H_{11}Br$
Isoamyl bromide
1-Bromo-3-methylbutane
RN: 107-82-4 **MP** (°C)**:** –112
MW: 151.05 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.324E-03	2.000E-01	16	F300	1 0 0 0 1	
1.300E-03	1.964E-01	16.5	F001	1 0 1 0 2	

507. $C_5H_{11}NO$
Pentanamide
Valeramide
RN: 626-97-1 **MP** (°C)**:** 102–104
MW: 101.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-01	5.594E+01	6	H059	0 0 0 0 0	
6.360E-01	6.433E+01	16	H059	0 0 0 0 0	
7.880E-01	7.971E+01	25	H059	0 0 0 0 0	
1.108E+00	1.121E+02	37	H059	0 0 0 0 0	

508. $C_5H_{11}NO_2$
DL-Valine
DL-Valin
RN: 516-06-3 **MP** (°C)**:** 296
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-01	6.552E+01	0	D018	2 2 2 1 2	
5.711E-01	6.690E+01	25	C018	0 0 0 0 0	
6.035E-01	7.070E+01	25	D016	1 0 0 0 2	
5.912E-01	6.926E+01	25	D018	2 2 2 1 2	
5.614E-01	6.577E+01	25	D041	1 0 0 0 2	
5.975E-01	7.000E+01	25	F300	1 0 0 0 0	
7.352E-01	8.612E+01	50	D018	2 2 2 1 2	
7.170E-01	8.400E+01	50	F300	1 0 0 0 1	
1.003E+00	1.175E+02	75	D018	2 2 2 1 2	
9.559E-01	1.120E+02	75	D041	1 0 0 0 2	
9.560E-01	1.120E+02	75	F300	1 0 0 0 2	
1.349E+00	1.580E+02	100	F300	1 0 0 0 2	
1.351E+00	1.583E+02	99.99	P349	0 0 0 0 0	

509. $C_5H_{11}NO_2$
L-Norvaline
L-(+)-2-Aminovaleric acid
RN: 6600-40-4 **MP** (°C)**:** >300
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.286E-01	9.707E+01	15	D041	1 0 0 0 2	

510. $C_5H_{11}NO_2$
tert-Butyl carbamate
O-t-Butyl carbamate
RN: 4248-19-5 **MP** (°C)**:** 105
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.250E+00	1.464E+02	37	H006	1 2 2 1 2	
1.259E+00	1.475E+02	ns	R424	0 0 0 0 0	

511. $C_5H_{11}NO_2$
n-Butyl carbamate
Butyl carbamate
RN: 592-35-8 **MP** (°C)**:** 51
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.577E+01	37	H006	1 2 2 1 1	

512. $C_5H_{11}NO_2$
Isobutyl carbamate
iso-Butyl carbamate
RN: 543-28-2 **MP** (°C)**:** 67
MW: 117.15 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-01	5.857E+01	37	H006	1 2 2 1 0	

513. $C_5H_{11}NO_2$
DL-Isovaline
DL-Isovalin
RN: 595-39-1 **MP** (°C)**:** 315
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E+00	2.809E+02	20	F300	1 0 0 0 2	

514. $C_5H_{11}NO_2$

D-Valine
β-Amino-isovalerian-saeure
β-Aminoisovaleric acid

RN: 640-68-6 **MP** (°C)**:** >295
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-02	1.512E+00	10	D038	1 0 1 0 0	EFG, unit assumed, *sic*
4.296E-01	5.033E+01	20	D041	1 0 0 0 1	
7.053E-01	8.263E+01	25	C018	0 0 0 0 0	
1.343E-02	1.574E+00	25	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.384E-02	1.622E+00	33	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.426E-02	1.671E+00	40	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.455E-02	1.705E+00	49	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.500E-02	1.757E+00	57	D038	1 0 1 0 0	EFG, unit assumed, *sic*
1.592E-02	1.865E+00	65	D038	1 0 1 0 0	EFG, unit assumed, *sic*

515. $C_5H_{11}NO_2$

Betaine
Betain

RN: 107-43-7 **MP** (°C)**:** 296
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E+00	6.110E+02	19.30	F300	1 0 0 0 2	

516. $C_5H_{11}NO_2$

DL-Norvaline
DL-2-Aminovaleric acid

RN: 760-78-1 **MP** (°C)**:** 303.0
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.251E-01	9.666E+01	15	D041	1 0 0 0 2	
7.768E-01	9.100E+01	18	F300	1 0 0 0 1	
6.616E-01	7.751E+01	25	K031	2 1 2 1 2	

517. $C_5H_{11}NO_2$

L-Valine
Valine
L-(+)-valine
L-2-Amino-3-methylbutyric acid
2-Amino-3-methylbutyric acid

RN: 72-18-4 **MP** (°C)**:** 315
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.180E-01	8.411E+01	15	D349	2 1 1 2 2	
4.866E-01	5.701E+01	20	B032	1 2 2 1 2	
7.360E-01	8.622E+01	20	D349	2 1 1 2 2	
4.992E-01	5.848E+01	25	B032	1 2 2 1 2	
6.940E-01	8.130E+01	25	D041	1 0 0 0 2	
7.550E-01	8.845E+01	25	D349	2 1 1 2 2	
4.710E-01	5.518E+01	25	G092	2 1 1 1 1	
4.710E-01	5.518E+01	25	G315	0 0 0 0 0	
5.900E-01	6.912E+01	25	N001	0 0 0 0 0	EFG
4.740E-01	5.553E+01	25	N012	2 0 2 1 2	
5.019E-01	5.880E+01	27	D036	0 0 0 0 0	
5.114E-01	5.991E+01	29.80	B032	1 2 2 1 2	
7.929E-01	9.289E+01	65	D041	1 0 0 0 2	

518. $C_5H_{11}NO_2$

3-Nitropentane
Pentane, 3-nitro-

RN: 551-88-2 **MP** (°C)**:**
MW: 117.15 **BP** (°C)**:** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.300E+00	25	A049	1 0 0 0 1	

519. $C_5H_{11}NO_2S$

DL-Methionine
DL-Methionin
DL-2-Amino-4-(methylthio)butyric acid
Acimetion

RN: 59-51-8 **MP** (°C)**:** 281
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	1.790E+01	0	F300	1 0 0 0 2	
1.905E-01	2.843E+01	19.99	F419	0 0 0 0 0	pH 5.81
2.191E-01	3.269E+01	25	D041	1 0 0 0 2	
2.191E-01	3.270E+01	25	F300	1 0 0 0 2	
3.039E-01	4.535E+01	39.99	F419	0 0 0 0 0	pH 5.56

(*continued*)

519. $C_5H_{11}NO_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.211E-01	4.791E+01	44.99	F419	0 0 0 0 0	pH 5.51
3.833E-01	5.720E+01	50	F300	1 0 0 0 2	
4.241E-01	6.328E+01	54.99	F419	0 0 0 0 0	pH 5.39
5.596E-01	8.350E+01	69.99	F419	0 0 0 0 0	pH 5.24
6.379E-01	9.519E+01	75	D041	1 0 0 0 2	
6.380E-01	9.520E+01	75	F300	1 0 0 0 2	
6.965E-01	1.039E+02	79.99	F419	0 0 0 0 0	pH 5.15
1.003E+00	1.497E+02	100	F300	1 0 0 0 2	
2.212E-01	3.300E+01	ns	K444	0 0 0 0 0	

520. $C_5H_{11}NO_2S$

Methionine
L-(–)-Methionine
2-Amino-4-(methylthio)butanoic acid
RN: 63-68-3 **MP** (°C)**:** –279
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.504E-01	5.228E+01	20	B032	1 2 2 1 2	
3.791E-01	5.656E+01	25	B032	1 2 2 1 2	
3.566E-01	5.321E+01	25	G315	0 0 0 0 0	
3.753E-01	5.600E+01	25.1	N024	0 0 0 0 0	
3.746E-01	5.590E+01	25.1	N026	0 0 0 0 0	
3.548E-01	5.294E+01	25.1	N027	1 1 2 2 2	
3.498E-01	5.220E+01	27	D036	0 0 0 0 0	
4.093E-01	6.107E+01	29.80	B032	1 2 2 1 2	

521. $C_5H_{11}NO_2S$

Penicillamine
3,3-Dimethyl-D-(–)-cysteine
D-3-Mercaptovaline
D-Penicillamine
RN: 52-67-5 **MP** (°C)**:** 198.0
MW: 149.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.702E-01	1.000E+02	20	C120	0 0 0 0 0	

522. $C_5H_{11}NO_2.H_2O$

Betaine (monohydrate)
Trimethylammonioacetate (monohydrate)
RN: 590-47-6 **MP** (°C)**:**
MW: 135.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E+00	6.109E+02	19	D041	1 0 0 0 2	

523. C_5H_{12}

Pentane
n-Pentane
RN: 109-66-0 **MP** (°C)**:** –130
MW: 72.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.106E-04	6.570E-02	0	P003	2 2 2 2 2	
5.666E-04	4.088E-02	4.0	N004	1 1 2 2 2	
1.516E-04	1.094E-02	4.8	L007	2 1 1 2 2	
1.516E-04	1.094E-02	5.1	L007	2 0 1 1 2	
5.944E-04	4.289E-02	10.0	N004	1 1 2 2 2	
1.635E-04	1.180E-02	14.8	L007	2 1 1 2 2	
2.425E-04	1.750E-02	20	M337	2 1 2 2 2	
5.444E-04	3.928E-02	20.0	N004	1 1 2 2 2	
1.563E-04	1.128E-02	24.8	L007	2 1 1 2 2	
5.267E-04	3.800E-02	25	A049	1 0 0 0 1	
5.475E-04	3.950E-02	25	K119	1 0 0 0 2	
5.336E-04	3.850E-02	25	M001	2 1 2 2 2	
5.336E-04	3.850E-02	25	M002	2 1 2 2 2	
5.650E-04	4.077E-02	25	M342	1 0 1 1 2	
6.597E-04	4.760E-02	25	P003	2 2 2 2 2	
5.611E-04	4.048E-02	25.0	N004	1 1 2 2 2	
5.475E-04	3.950E-02	25.0	P051	2 1 1 2 2	
5.475E-04	3.950E-02	25.00	P007	2 1 2 2 2	
5.611E-04	4.048E-02	30.0	N004	1 1 2 2 2	
1.509E-04	1.089E-02	34.8	L007	2 1 1 2 2	
5.516E-04	3.980E-02	40.1	P051	2 1 1 2 2	
5.516E-04	3.980E-02	40.10	P007	2 1 2 2 2	
5.793E-04	4.180E-02	55.7	P051	2 1 1 2 2	
5.793E-04	4.180E-02	55.70	P007	2 1 2 2 2	
9.619E-04	6.940E-02	99.1	P051	2 1 1 2 2	
9.619E-04	6.940E-02	99.10	P007	2 1 2 2 2	
1.525E-03	1.100E-01	121.3	P051	2 1 1 2 2	
1.525E-03	1.100E-01	121.30	P007	2 1 2 2 2	
2.786E-03	2.010E-01	137.3	P051	2 1 1 2 2	
2.786E-03	2.010E-01	137.30	P007	2 1 2 2 2	
4.130E-03	2.980E-01	149.5	P051	2 1 1 2 2	
4.130E-03	2.980E-01	149.50	P007	2 1 2 2 2	
1.010E-04	7.287E-03	ns	D348	0 0 0 0 0	

524. C_5H_{12}
2-Methylbutane
Isopentane
Izopentan
RN: 78-78-4 **MP** (°C)**:** –160
MW: 72.15 **BP** (°C)**:** 30

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	7.240E-02	0	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	K119	1 0 0 0 2	
6.625E-04	4.780E-02	25	M001	2 1 2 2 2	
6.625E-04	4.780E-02	25	M002	2 1 2 2 2	
6.874E-04	4.960E-02	25	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	P007	2 1 2 2 2	
6.653E-04	4.800E-02	25	P051	2 1 1 2 2	

525. C_5H_{12}
Neopentane
2,2-Dimethylpropane
RN: 463-82-1 **MP** (°C)**:**
MW: 72.15 **BP** (°C)**:** 9.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-04	1.602E-02	25	D346	0 0 0 0 0	
4.601E-04	3.320E-02	25	M001	2 1 2 2 2	
5.611E-04	4.048E-02	25	S212	2 1 2 2 2	
3.833E-04	2.766E-02	40	S212	2 1 2 2 1	
2.667E-04	1.924E-02	60	S212	2 1 2 2 1	
2.389E-04	1.724E-02	80	S212	2 1 2 2 1	

526. $C_5H_{12}ClO_2PS_2$
Chlormephos
Dotan
Diethyl *S*-(chloromethyl) dithiophosphate
RN: 24934-91-6 **MP** (°C)**:**
MW: 234.70 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-04	6.000E-02	20	L303	1 0 0 0 1	
2.556E-04	6.000E-02	20	M161	1 0 0 0 1	
2.559E-04	6.005E-02	ns	S460	0 0 0 0 0	

527. $C_5H_{12}NO_3PS_2$
Dimethoate
O,O-Dimethyl *S*-(*N*-methylcarbamoylmethyl) dithiophosphate
RN: 60-51-5 **MP** (°C)**:** 52.25
MW: 229.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	2.514E+01	20	B179	0 0 0 0 0	
1.309E-01	3.000E+01	20	G319	0 0 0 0 0	
1.090E-01	2.500E+01	21	M161	1 0 0 0 1	
1.701E-01	3.900E+01	ns	M061	0 0 0 0 1	

528. $C_5H_{12}N_2$
2-Methylpiperazine
2-Methyl-piperazin
RN: 109-07-9 **MP** (°C)**:** 66
MW: 100.16 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.343E+00	4.350E+02	20	F300	1 0 0 0 2	

529. $C_5H_{12}N_2O$
Methyl-*n*-butylnitrosamine
MBN
RN: 7068-83-9 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-01	2.323E+01	24	M031	1 1 1 1 1	

530. $C_5H_{12}O$
2-Methyl-1-butanol
DL-2-Methyl-1-butanol
2-Methylbutan-1-ol
RN: 137-32-6 **MP** (°C)**:** –70
MW: 88.15 **BP** (°C)**:** 128.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.269E-01	3.763E+01	.5	S307	1 1 0 2 2	
3.720E-01	3.279E+01	9.7	S307	1 1 0 2 2	
3.122E-01	2.752E+01	19.6	S307	1 1 0 2 2	
3.496E-01	3.082E+01	20	G004	2 2 2 2 2	
3.304E-01	2.913E+01	25	C093	2 1 1 1 1	
3.272E-01	2.884E+01	25	G004	2 2 2 2 2	
2.778E-01	2.449E+01	29.6	S307	1 1 0 2 2	
3.122E-01	2.752E+01	30	G004	2 2 2 2 2	

(*continued*)

530. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.616E-01	2.306E+01	39.3	S307	1 1 0 2 2	
2.453E-01	2.162E+01	49.6	S307	1 1 0 2 2	
2.301E-01	2.028E+01	59.3	S307	1 1 0 2 2	
2.485E-01	2.191E+01	69.5	S307	1 1 0 2 2	
2.551E-01	2.248E+01	79.7	S307	1 1 0 2 2	
2.724E-01	2.401E+01	90.8	S307	1 1 0 2 2	

531. $C_5H_{12}O$

tert-Isoamyl alcohol
3-Methyl-1-butanol
Isopentyl alcohol
Isoamyl alcohol

RN: 123-51-3 **MP** (°C)**:** –117
MW: 88.15 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.079E-01	3.596E+01	0	S307	1 1 0 2 2	
3.090E-01	2.724E+01	10	A328	0 0 0 0 0	
3.454E-01	3.044E+01	10.1	S307	1 1 0 2 2	
3.347E-01	2.950E+01	15	K002	1 2 1 1 2	
3.130E-01	2.759E+01	18	F001	1 0 1 2 2	
2.918E-01	2.572E+01	19.8	S307	1 1 0 2 2	
3.120E-01	2.750E+01	20	F300	1 0 0 0 2	
3.144E-01	2.771E+01	20	G004	2 2 2 2 2	
3.111E-01	2.743E+01	20	K002	1 2 1 1 2	
9.586E-01	8.450E+01	20	K085	1 0 0 0 2	
2.659E-01	2.344E+01	25	A328	0 0 0 0 0	
3.411E-01	3.007E+01	25	C068	2 2 2 1 2	
2.982E-01	2.629E+01	25	C093	2 1 1 1 1	
3.251E-01	2.865E+01	25	F317	2 1 1 1 2	
2.950E-01	2.601E+01	25	G004	2 2 2 2 2	
2.950E-01	2.601E+01	25	K002	1 2 1 1 2	
2.799E-01	2.468E+01	30	G004	2 2 2 2 2	
2.832E-01	2.496E+01	30	K002	1 2 1 1 2	
2.842E-01	2.506E+01	30.1	H043	2 2 2 2 2	average of 3
2.540E-01	2.239E+01	30.2	S307	1 1 0 2 2	
2.442E-01	2.153E+01	40	A328	0 0 0 0 0	
2.420E-01	2.133E+01	40.0	S307	1 1 0 2 2	
2.257E-01	1.990E+01	49.9	S307	1 1 0 2 2	
2.431E-01	2.143E+01	59.8	S307	1 1 0 2 2	
2.344E-01	2.066E+01	70.0	S307	1 1 0 2 2	
2.442E-01	2.153E+01	80.0	S307	1 1 0 2 2	
2.518E-01	2.220E+01	90.0	S307	1 1 0 2 2	
2.836E-01	2.500E+01	ns	L003	0 0 2 1 2	
2.767E-01	2.439E+01	rt	H111	0 0 0 0 1	

532. $C_5H_{12}O$
Neopentyl alcohol
t-Butyl carbinol
RN: 75-84-3 **MP** (°C)**:** 53
MW: 88.15 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.048E-01	3.568E+01	12.0	S307	1 1 0 2 2	
3.826E-01	3.372E+01	18.8	S307	1 1 0 2 2	
4.090E-01	3.605E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	G004	2 2 2 2 2	
3.603E-01	3.176E+01	30	G004	2 2 2 2 2	
3.229E-01	2.847E+01	30.0	S307	1 1 0 2 2	
2.982E-01	2.629E+01	40.0	S307	1 1 0 2 2	
2.616E-01	2.306E+01	50.0	S307	1 1 0 2 2	
2.778E-01	2.449E+01	60.0	S307	1 1 0 2 2	
2.399E-01	2.114E+01	70.2	S307	1 1 0 2 2	
2.864E-01	2.525E+01	80.0	S307	1 1 0 2 2	
2.637E-01	2.325E+01	90.0	S307	1 1 0 2 2	

533. $C_5H_{12}O$
Methyl *tert*-butyl ether
tert-Butyl methyl ether
RN: 1634-04-4 **MP** (°C)**:** –109
MW: 88.15 **BP** (°C)**:** 54.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.564E-01	5.786E+01	2.34	S461	0 0 0 0 0	
6.236E-01	5.497E+01	9.99	S461	0 0 0 0 0	
5.196E-01	4.580E+01	20	E019	1 0 1 1 1	
4.738E-01	4.177E+01	24.99	S461	0 0 0 0 0	
5.815E-01	5.126E+01	25	K072	1 0 1 1 1	
5.815E-01	5.126E+01	25	M087	1 1 2 1 2	

534. $C_5H_{12}O$
3-Pentanol
Pentan-3-ol
Diethyl carbinol
RN: 584-02-1 **MP** (°C)**:** <25
MW: 88.15 **BP** (°C)**:** 115.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.704E-01	7.672E+01	0	S307	1 1 0 2 2	
7.382E-01	6.507E+01	10.2	S307	1 1 0 2 2	
6.026E-01	5.312E+01	20	G004	2 2 2 2 2	

(*continued*)

534. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-01	5.536E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	25	C093	2 1 1 1 1	
5.556E-01	4.898E+01	25	G004	2 2 2 2 2	
5.144E-01	4.535E+01	30	G004	2 2 2 2 2	
5.730E-01	5.051E+01	30.0	S307	1 1 0 2 2	
4.510E-01	3.975E+01	40.0	S307	1 1 0 2 2	
4.604E-01	4.058E+01	50.0	S307	1 1 0 2 2	
3.889E-01	3.428E+01	60.0	S307	1 1 0 2 2	
3.783E-01	3.335E+01	70.0	S307	1 1 0 2 2	
3.635E-01	3.204E+01	80.0	S307	1 1 0 2 2	
3.773E-01	3.326E+01	90.0	S307	1 1 0 2 2	
1.392E+00	1.227E+02	ns	L003	0 0 2 1 1	
5.196E-01	4.580E+01	rt	H111	0 0 0 0 1	

535. $C_5H_{12}O$

3-Methyl-2-butanol
Methylisopropylcarbinol

RN: 598-75-4 **MP** (°C)**:** <25
MW: 88.15 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.771E-01	7.732E+01	0	S307	1 1 0 2 2	
7.609E-01	6.708E+01	10.1	S307	1 1 0 2 2	
6.492E-01	5.723E+01	20	G004	2 2 2 2 2	
6.381E-01	5.625E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	30	G004	2 2 2 2 2	
5.536E-01	4.880E+01	30.0	S307	1 1 0 2 2	
4.833E-01	4.260E+01	40.0	S307	1 1 0 2 2	
4.416E-01	3.892E+01	50.0	S307	1 1 0 2 2	
3.720E-01	3.279E+01	60.0	S307	1 1 0 2 2	
4.005E-01	3.531E+01	70.0	S307	1 1 0 2 2	
3.942E-01	3.475E+01	79.5	S307	1 1 0 2 2	
3.942E-01	3.475E+01	90.0	S307	1 1 0 2 2	

536. $C_5H_{12}O$

Ethylisopropyl ether
Propane, 2-ethoxy-

RN: 625-54-7 **MP** (°C)**:**
MW: 88.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.409E+01	ns	J300	0 0 0 0 0	

537. $C_5H_{12}O$

1-Pentanol
Amyl alcohol
Pentanol
Pentyl alcohol
n-Amyl alcohol

RN: 71-41-0 **MP** (°C)**:** –79
MW: 88.15 **BP** (°C)**:** 138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.321E-01	3.809E+01	–.5	F051	2 1 0 1 2	
3.358E-01	2.960E+01	0	E029	1 2 0 1 2	
3.635E-01	3.204E+01	0	S307	1 1 0 2 2	
3.709E-01	3.269E+01	7	F051	2 1 0 1 2	
2.982E-01	2.629E+01	10	E029	1 2 0 1 2	
2.864E-01	2.525E+01	10.2	S307	1 1 0 2 2	
3.068E-01	2.705E+01	14	F051	2 1 0 1 2	
3.004E-01	2.648E+01	15	F051	2 1 0 1 2	
5.395E+00	4.756E+02	15.5	F051	2 1 0 1 2	
2.875E-01	2.534E+01	16.5	F051	2 1 0 1 2	
2.821E-01	2.487E+01	18	F051	2 1 0 1 2	
2.453E-01	2.162E+01	20	A015	1 2 1 1 2	
1.020E-02	8.992E-01	20	D052	1 1 0 0 0	*sic*
2.605E-01	2.296E+01	20	E029	1 2 0 1 2	
2.616E-01	2.306E+01	20	G004	2 2 2 2 2	
1.676E-01	1.478E+01	20	L049	1 1 2 1 1	
3.070E-01	2.706E+01	20	M312	1 0 0 0 1	
2.496E-01	2.200E+01	20.2	S307	1 1 0 2 2	
3.607E-01	3.180E+01	22	H072	1 0 1 1 2	
2.691E-01	2.372E+01	23	F051	2 1 0 1 2	
3.730E-01	3.288E+01	25	B019	1 0 1 2 0	
2.451E-01	2.160E+01	25	B038	1 0 1 1 2	
1.896E-01	1.672E+01	25	B060	2 0 1 1 1	
2.442E-01	2.153E+01	25	C093	2 1 1 1 1	
1.000E+00	8.815E+01	25	F044	1 0 0 0 0	EFG
2.137E-01	1.884E+01	25	F317	2 1 1 1 2	
2.431E-01	2.143E+01	25	G004	2 2 2 2 2	
2.300E-01	2.027E+01	25	G075	1 0 1 0 1	
2.810E-01	2.477E+01	25	H028	2 0 2 0 2	
2.817E-01	2.483E+01	25	H104	1 0 0 0 1	
2.500E-01	2.204E+01	25	K025	2 2 1 1 1	
2.561E-01	2.258E+01	29	F051	2 1 0 1 2	
2.333E-01	2.057E+01	30	E029	1 2 0 1 2	
2.257E-01	1.990E+01	30	G004	2 2 2 2 2	
2.246E-01	1.980E+01	30.6	S307	1 1 0 2 2	
5.368E+00	4.732E+02	34.0	F051	2 1 0 1 2	
2.475E-01	2.181E+01	36	F051	2 1 0 1 2	
2.130E-01	1.878E+01	37	E028	1 0 1 1 2	
2.115E-01	1.865E+01	40	E029	1 2 0 1 2	
2.082E-01	1.836E+01	40.2	S307	1 1 0 2 2	
2.006E-01	1.768E+01	50	E029	1 2 0 1 2	

(*continued*)

537. $C_5H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-01	1.797E+01	50.0	S307	1 1 0 2 2	
2.475E-01	2.181E+01	58	F051	2 1 0 1 2	
2.006E-01	1.768E+01	60	E029	1 2 0 1 2	
2.039E-01	1.797E+01	60.3	S307	1 1 0 2 2	
5.290E+00	4.664E+02	69.5	F051	2 1 0 1 2	
2.061E-01	1.816E+01	70	E029	1 2 0 1 2	
2.170E-01	1.913E+01	70.0	S307	1 1 0 2 2	
2.561E-01	2.258E+01	72.0	F051	2 1 0 1 2	
2.115E-01	1.865E+01	80	E029	1 2 0 1 2	
2.213E-01	1.951E+01	80.0	S307	1 1 0 2 2	
2.691E-01	2.372E+01	81	F051	2 1 0 1 2	
2.821E-01	2.487E+01	87	F051	2 1 0 1 2	
2.224E-01	1.961E+01	90	E029	1 2 0 1 2	
2.453E-01	2.162E+01	90.7	S307	1 1 0 2 2	
2.875E-01	2.534E+01	91	F051	2 1 0 1 2	
3.004E-01	2.648E+01	95	F051	2 1 0 1 2	
5.180E+00	4.566E+02	97.3	F051	2 1 0 1 2	
3.068E-01	2.705E+01	98	F051	2 1 0 1 2	
2.496E-01	2.200E+01	100	E029	1 2 0 1 2	
2.875E-01	2.534E+01	110	E029	1 2 0 1 2	
3.709E-01	3.269E+01	112	F051	2 1 0 1 2	
3.304E-01	2.913E+01	120	E029	1 2 0 1 2	
5.048E+00	4.450E+02	122.3	F051	2 1 0 1 2	
4.321E-01	3.809E+01	126	F051	2 1 0 1 2	
3.889E-01	3.428E+01	130	E029	1 2 0 1 2	
4.677E-01	4.123E+01	140	E029	1 2 0 1 2	
5.351E-01	4.717E+01	140	F051	2 1 0 1 2	
4.896E+00	4.316E+02	141.6	F051	2 1 0 1 2	
5.853E-01	5.159E+01	145	F051	2 1 0 1 2	
6.290E-01	5.545E+01	148.5	F051	2 1 0 1 2	
5.761E-01	5.078E+01	150	E029	1 2 0 1 2	
4.707E+00	4.149E+02	157.3	F051	2 1 0 1 2	
7.322E-01	6.455E+01	160	E029	1 2 0 1 2	
9.060E-01	7.987E+01	167.0	F051	2 1 0 1 2	
9.889E-01	8.717E+01	170	E029	1 2 0 1 2	
1.001E+00	8.826E+01	171.2	F051	2 1 0 1 2	
4.374E+00	3.856E+02	174.0	F051	2 1 0 1 2	
1.690E+00	1.489E+02	180	E029	1 2 0 1 2	
4.089E+00	3.605E+02	181.3	F051	2 1 0 1 2	
1.435E+00	1.265E+02	182.5	F051	2 1 0 1 2	
3.774E+00	3.327E+02	185.2	F051	2 1 0 1 2	
1.833E+00	1.616E+02	186.0	F051	2 1 0 1 2	
2.270E+00	2.001E+02	186.5	F051	2 1 0 1 2	
3.472E+00	3.061E+02	186.5	F051	2 1 0 1 2	
3.237E+00	2.854E+02	187.4	F051	2 1 0 1 2	
3.040E+00	2.680E+02	187.5	F051	2 1 0 1 2	
2.810E-01	2.477E+01	ns	A406	0 0 0 0 1	
2.538E-01	2.237E+01	ns	L003	0 0 2 1 2	
2.224E-01	1.961E+01	rt	H111	0 0 0 0 1	

538. $C_5H_{12}O$

2-Pentanol
iso-Amyl alcohol
sec-Amyl alcohol
Methyl propyl carbinol

RN: 6032-29-7 **MP** (°C)**:** –50
MW: 88.15 **BP** (°C)**:** 119.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.708E-01	6.795E+01	0	S307	1 1 0 2 2	
6.189E-01	5.455E+01	10.1	S307	1 1 0 2 2	
5.030E-01	4.434E+01	19.5	S307	1 1 0 2 2	
4.573E-01	4.031E+01	20	C042	0 0 0 0 0	
1.473E-02	1.298E+00	20	D052	1 1 0 0 0	*sic*
4.538E-01	4.000E+01	20	F300	1 0 0 0 1	
5.258E-01	4.635E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	B019	1 0 1 2 0	
4.843E-01	4.270E+01	25	G004	2 2 2 2 2	
4.499E-01	3.966E+01	30	G004	2 2 2 2 2	
4.300E-01	3.791E+01	30.6	S307	1 1 0 2 2	
3.900E-01	3.438E+01	40.0	S307	1 1 0 2 2	
3.645E-01	3.213E+01	50.0	S307	1 1 0 2 2	
3.432E-01	3.026E+01	60.0	S307	1 1 0 2 2	
3.379E-01	2.979E+01	70.1	S307	1 1 0 2 2	
3.443E-01	3.035E+01	79.9	S307	1 1 0 2 2	
3.368E-01	2.969E+01	90.3	S307	1 1 0 2 2	
5.149E-01	4.539E+01	ns	L003	0 0 2 1 2	

539. $C_5H_{12}O$

tert-Pentyl alcohol
Dimethylethylcarbinol
tert-Amylalkohol

RN: 75-85-4 **MP** (°C)**:**
MW: 88.15 **BP** (°C)**:** 102.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.548E+00	1.364E+02	.5	S307	1 1 0 2 2	
1.462E+00	1.289E+02	9.8	S307	1 1 0 2 2	
1.259E+00	1.110E+02	20	F300	1 0 0 0 2	
1.229E+00	1.083E+02	20	G004	2 2 2 2 2	
1.170E+00	1.031E+02	20.8	S307	1 1 0 2 2	
1.124E+00	9.910E+01	25	G004	2 2 2 2 2	
5.965E-01	5.258E+01	25	G004	2 2 2 2 2	
1.026E+00	9.041E+01	29.5	S307	1 1 0 2 2	
1.041E+00	9.173E+01	30	G004	2 2 2 2 2	
8.549E-01	7.536E+01	39.5	S307	1 1 0 2 2	
7.649E-01	6.743E+01	49.0	S307	1 1 0 2 2	
6.673E-01	5.882E+01	60.0	S307	1 1 0 2 2	
6.391E-01	5.634E+01	70.2	S307	1 1 0 2 2	
6.117E-01	5.393E+01	80.1	S307	1 1 0 2 2	
5.883E-01	5.186E+01	90.2	S307	1 1 0 2 2	
1.124E+00	9.910E+01	rt	H111	0 0 0 0 2	

540. $C_5H_{12}O_2$
Formaldehyde diethyl acetal
Diethoxymethane
Diethylacetalformaldehyde
Formaldehyd-diaethyl-acetal
RN: 462-95-3 **MP** (°C)**:**
MW: 104.15 **BP** (°C)**:** 87.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.721E-01	7.000E+01	18	F300	1 0 0 0 1	

541. $C_5H_{12}O_4$
Pentaerythritol
2,2-bis(Hydroxymethyl)-1,3-propanediol
PE 200
Tetramethylolmethane
RN: 115-77-5 **MP** (°C)**:** 260
MW: 136.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-01	3.846E+01	0	M043	1 0 0 0 0	
3.498E-01	4.762E+01	10	M043	1 0 0 0 0	
3.863E-01	5.260E+01	15	F300	1 0 0 0 2	
4.157E-01	5.660E+01	20	M043	1 0 0 0 0	
5.441E-01	7.407E+01	30	M043	1 0 0 0 0	
8.450E-01	1.150E+02	40	M043	1 0 0 0 1	
1.324E+00	1.803E+02	60	M043	1 0 0 0 1	
2.099E+00	2.857E+02	80	M043	1 0 0 0 1	
3.672E+00	5.000E+02	100	M043	1 0 0 0 2	
3.890E-01	5.297E+01	ns	R424	0 0 0 0 0	

542. $C_5H_{12}O_5$
Adonitol
Adonit
Adonite
RN: 488-81-3 **MP** (°C)**:** 104
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E+00	6.016E+02	25	C346	0 0 0 0 0	

543. $C_5H_{12}O_5$
Xylitol
RN: 87-99-0 **MP** (°C)**:** 96 K
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.798E+00	5.778E+02	20.12	W414	0 0 0 0 0	
3.963E+00	6.030E+02	25.1	W414	0 0 0 0 0	
4.153E+00	6.319E+02	30.01	W414	0 0 0 0 0	
4.355E+00	6.627E+02	35.05	W414	0 0 0 0 0	
4.550E+00	6.922E+02	40.13	W414	0 0 0 0 0	
4.721E+00	7.183E+02	45.10	W414	0 0 0 0 0	
4.873E+00	7.414E+02	50.09	W414	0 0 0 0 0	
5.001E+00	7.610E+02	55.05	W414	0 0 0 0 0	

544. $C_5H_{12}O_5$
DL-Arabinitol
(±)-Arabitol
RN: 2152-56-9 **MP** (°C)**:** 103
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.459E+00	6.785E+02	25	C346	0 0 0 0 0	

545. $C_5H_{13}N$
N-Methyldiethylamine
N,N-Diethylmethylamine
RN: 616-39-7 **MP** (°C)**:**
MW: 87.17 **BP** (°C)**:** 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E+00	3.105E+02	49.40	C086	2 2 2 2 2	average of 5
4.453E+00	3.881E+02	49.50	C086	2 2 2 2 2	
2.236E+00	1.949E+02	49.80	C086	2 2 2 2 2	
5.715E+00	4.982E+02	50.50	C086	2 2 2 2 2	
1.581E+00	1.378E+02	51.20	C086	2 2 2 2 2	
1.413E+00	1.231E+02	52.00	C086	2 2 2 2 2	
6.981E+00	6.085E+02	53.10	C086	2 2 2 2 2	
7.246E+00	6.316E+02	54.00	C086	2 2 2 2 2	

546. $C_5H_{13}O_3PS_2$
Demephion
O,O-Dimethyl 2-methylmercaptoethyl thiophosphate
Thiolo-tinox
RN: 8065-62-1 **MP** (°C)**:**
MW: 216.26 **BP** (°C)**:** 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.312E-03	5.000E-01	20	M061	1 0 0 0 2	form II
9.248E-03	2.000E+00	ns	M061	0 0 0 0 2	form I
1.387E-02	3.000E+00	rt	M161	0 0 0 0 0	form II
1.387E-03	3.000E-01	rt	M161	0 0 0 0 2	form I

547. C_5Cl_6
Hexachlorocyclopentadiene
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene
Hexachloro-1,3-cyclopentadiene
1,2,3,4,5,5-Hexachlorocyclopentadiene
RN: 77-47-4 **MP** (°C)**:** –9.9
MW: 272.77 **BP** (°C)**:** 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-06	8.050E-04	22.5	G301	0 0 0 0 0	

548. $C_6HCl_3N_2S$
4,5,7-Trichloro-2,1,3-benzothiadiazole
PH 40-21
TH 052 H
RN: 1982-55-4 **MP** (°C)**:** 131.5
MW: 239.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.263E-06	1.500E-03	10	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	M061	1 0 0 0 1	
1.795E-05	4.300E-03	30	B200	1 0 0 0 1	

549. $C_6HCl_4NO_2$
2,3,4,5-Tetrachloronitrobenzene
1,2,3,4-Tetrachloro-5-nitrobenzene
2,3,4,5-Tetrachloro-1-nitrobenzene
1-Nitro-2,3,4,5-tetrachlorobenzene
RN: 879-39-0 **MP** (°C)**:** 66.0
MW: 260.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.305E-03	20	E308	1 2 2 1 1	

550. $C_6HCl_4NO_2$
2,3,4,6-Tetrachloronitrobenzene
Benzene, 1,2,3,5-tetrachloro-4-nitro-
RN: 3714-62-3 **MP** (°C)**:**
MW: 260.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-05	7.566E-03	20	E308	1 2 2 1 1	

551. $C_6HCl_4NO_2$
2,3,5,6-Tetrachloronitrobenzene
Tecnazene
RN: 117-18-0 **MP** (°C)**:** 99.5
MW: 260.89 **BP** (°C)**:** 304.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-06	2.087E-03	20	E308	1 2 2 1 0	

552. C_6HCl_5
Pentachlorobenzene
Penta-chlorobenzene
RN: 608-93-5 **MP** (°C)**:** 82
MW: 250.34 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-06	2.503E-04	20	K337	1 0 0 0 2	
9.550E-07	2.391E-04	22	K305	1 0 1 1 0	
1.538E-06	3.850E-04	23	C305	1 1 2 2 2	
5.320E-06	1.332E-03	25	B173	2 0 2 2 2	
2.600E-06	6.509E-04	25	B317	0 0 0 0 0	
3.320E-06	8.311E-04	25	M342	1 0 1 1 2	
3.320E-06	8.311E-04	ns	M308	0 0 1 1 2	

553. C_6HCl_5O
Pentachlorophenol
PCP
2,3,4,5,6-Pentachloro-phenol-
Phenol, 2,3,4,5,6-pentachloro-
Dowicide 7
Fungifen
RN: 87-86-5 **MP** (°C)**:** 174
MW: 266.34 **BP** (°C)**:** 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.877E-05	5.000E-03	0	C310	0 0 0 0 0	
1.877E-05	5.000E-03	0	G310	1 0 0 0 0	
1.877E-05	5.000E-03	0	M061	1 0 0 0 0	

(*continued*)

553. C_6HCl_5O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-05	1.400E-02	20	B185	0 0 0 0 0	
5.256E-05	1.400E-02	22.5	G301	0 0 0 0 0	
6.195E-05	1.650E-02	25	B183	0 0 0 0 1	
8.260E-05	2.200E-02	25	B185	0 0 0 0 0	
3.600E-05	9.588E-03	25	B316	0 0 0 0 0	
6.908E-05	1.840E-02	25	M373	1 0 2 1 2	
5.256E-05	1.400E-02	25	O320	0 0 0 0 0	
8.035E-05	2.140E-02	25.1	A400	2 1 2 2 2	
5.256E-05	1.400E-02	26.70	L095	2 2 1 1 2	
6.758E-05	1.800E-02	27	C310	0 0 0 0 0	
6.758E-05	1.800E-02	27	G310	1 0 0 0 1	
6.758E-05	1.800E-02	27	M061	1 0 0 0 1	
3.484E-03	9.280E-01	30	A400	2 1 2 2 2	
7.509E-05	2.000E-02	30	M161	1 0 0 0 1	
1.126E-04	3.000E-02	50	B200	1 0 0 0 0	
1.314E-04	3.500E-02	50	C310	0 0 0 0 0	
1.314E-04	3.500E-02	50	G310	1 0 0 0 1	
1.314E-04	3.500E-02	50	M061	1 0 0 0 1	
2.178E-04	5.800E-02	62	C310	0 0 0 0 0	
2.178E-04	5.800E-02	62	G310	1 0 0 0 1	
3.191E-04	8.499E-02	70	C310	0 0 0 0 0	
3.191E-04	8.499E-02	70	G310	1 0 0 0 1	
7.509E-05	2.000E-02	ns	L311	0 0 0 0 1	
7.134E-05	1.900E-02	ns	M110	0 0 0 0 0	EFG
6.007E-06	1.600E-03	ns	N013	0 0 0 0 1	

554. C_6HF_5O

Pentafluorophenol

PFP

RN: 771-61-9 **MP** (°C)**:** 34–36

MW: 184.07 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	5.522E+01	25	P031	0 0 0 0 0	

555. $C_6H_2Br_2ClNO_2$

2,6-Dibromoquinone-3-chlorimide

2,6-Dibromoquinonechloroimide

RN: **MP** (°C)**:**

MW: 315.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	6.307E-02	20	G043	1 0 1 1 0	

556. $C_6H_2Br_4$

1,2,4,5-Tetrabromobenzene

RN: 636-28-2 **MP** (°C)**:**
MW: 393.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.724E-08	1.860E-05	10	K440	0 0 0 0 0	
1.105E-07	4.350E-05	25	K440	0 0 0 0 0	
1.976E-07	7.780E-05	35	K440	0 0 0 0 0	

557. $C_6H_2ClN_3O_6$

2,4,6-Trinitro-1-chlorobenzene
Picryl chloride
2-Chlor-1,3,5-trinitrobenzol
Chlorure de picryle

RN: 88-88-0 **MP** (°C)**:**
MW: 247.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.190E-04	1.780E-01	15	D066	1 2 0 0 2	
7.189E-04	1.780E-01	15	D071	1 2 0 0 2	
7.271E-04	1.800E-01	15	F300	1 0 0 0 1	
2.141E-03	5.300E-01	16	D066	1 2 0 0 2	
2.140E-03	5.297E-01	50	D071	1 2 0 0 1	
1.398E-02	3.460E+00	100	D066	1 2 0 0 2	
1.393E-02	3.448E+00	100	D071	1 2 0 0 2	
1.454E-02	3.600E+00	100	F300	1 0 0 0 1	

558. $C_6H_2Cl_2O_4$

Chloranilic acid
Chloranilsaeure

RN: 87-88-7 **MP** (°C)**:** 283
MW: 208.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.091E-03	1.900E+00	14	F300	1 0 0 0 1	
6.699E-02	1.400E+01	99	F300	1 0 0 0 1	

559. $C_6H_2Cl_3NO_2$

2,4,5-Trichloronitrobenzene
1,2,4-Trichloro-5-nitrobenzene
2,4,5-Trichloro-1-nitrobenzene
1,4,5-Trichloro-2-nitrobenzene
3,4,6-Trichloronitrobenzene

RN: 89-69-0 **MP** (°C)**:** 57
MW: 226.45 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.944E-02	20	E308	1 2 2 1 2	

560. $C_6H_2Cl_3NO_2$
2,3,4-Trichloronitrobenzene
1,2,3-Trichloro-4-nitrobenzene
2,3,4-Trichloro-1-nitrobenzene
RN: 17700-09-3 **MP** (°C)**:** 55.5
MW: 226.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.604E-02	20	E308	1 2 2 1 2	

561. $C_6H_2Cl_4$
1,2,4,5-Tetrachlorobenzene
s-Tetrachlorobenzene
RN: 95-94-3 **MP** (°C)**:** 139
MW: 215.89 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.445E-06	3.121E-04	20	K337	1 0 0 0 2	
1.349E-06	2.912E-04	22	K305	1 0 1 1 1	
2.154E-06	4.650E-04	25	B304	2 0 2 2 2	
5.900E-06	1.274E-03	25	B317	0 0 0 0 0	
1.090E-05	2.353E-03	25	M342	1 0 1 1 2	
1.600E-06	3.454E-04	25.2	T428	0 0 0 0 0	
1.806E-06	3.900E-04	ns	B393	0 0 0 0 0	
1.090E-05	2.353E-03	ns	M308	0 0 1 1 2	

562. $C_6H_2Cl_4$
Trichlorobenzyl chloride
TCBC
RN: 1344-32-7 **MP** (°C)**:**
MW: 215.89 **BP** (°C)**:** 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.264E-06	2.000E-03	25	B200	1 0 0 0 0	

563. $C_6H_2Cl_4$
1,2,3,4-Tetrachlorobenzene
Benzene, 1,2,3,4-tetrachloro-
RN: 634-66-2 **MP** (°C)**:** 48
MW: 215.89 **BP** (°C)**:** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-05	3.422E-03	20	K337	1 0 0 0 2	
3.326E-05	7.180E-03	23	C305	1 1 2 2 2	
2.742E-05	5.920E-03	25	B304	2 0 2 2 2	
3.600E-05	7.772E-03	25	B317	0 0 0 0 0	
5.650E-05	1.220E-02	25	M342	1 0 1 1 2	
5.650E-05	1.220E-02	ns	M308	0 0 1 1 2	

564. $C_6H_2Cl_4$

1,2,3,5-Tetrachlorobenzene
1,2,4,6-Tetrachlorobenzene

RN: 634-90-2 **MP** (°C)**:** 50
MW: 215.89 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	2.159E-03	20	K337	1 0 0 0 2	
1.148E-05	2.479E-03	22	K305	1 0 1 1 2	
1.496E-05	3.230E-03	23	C305	1 1 2 2 2	
1.860E-05	4.016E-03	25	B173	2 0 2 2 2	
2.362E-05	5.100E-03	25	B304	2 0 2 2 2	
1.660E-05	3.584E-03	25	B317	0 0 0 0 0	
1.340E-05	2.893E-03	25	M342	1 0 1 1 2	
1.654E-05	3.570E-03	ns	H123	0 0 0 0 0	
1.340E-05	2.893E-03	ns	M308	0 0 1 1 2	

565. $C_6H_2Cl_4O$

2,3,4,6-Tetrachlorophenol
Phenol, 2,3,4,6-tetrachloro-
1-Hydroxy-2,3,4,6-tetrachlorobenzene
TCP

RN: 58-90-2 **MP** (°C)**:**
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.900E-04	1.832E-01	25	B316	0 0 0 0 0	

566. $C_6H_2Cl_4O$

2,3,4,5-Tetrachlorophenol
Phenol, 2,3,4,5-tetrachloro-

RN: 4901-51-3 **MP** (°C)**:** 116
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.158E-04	1.660E-01	25	M373	1 0 2 1 2	

567. $C_6H_2Cl_4O$

2,3,5,6-Tetrachlorophenol
Phenol, 2,3,5,6-tetrachloro-

RN: 935-95-5 **MP** (°C)**:** 115
MW: 231.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.312E-04	1.000E-01	25	M373	1 0 2 1 2	

568. $C_6H_2Cl_4O_2$
Tetrachlorohydroquinone
2,3,5,6-Tetrachlorohydroquinone
RN: 87-87-6 **MP** (°C)**:**
MW: 247.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.673E-05	2.150E-02	ns	L311	0 0 0 0 1	

569. $C_6H_2F_4$
1,2,4,5-Tetrafluorobenzene
2,3,5,6-Tetrafluorobenzene
p-Tetrafluorobenzene
RN: 327-54-8 **MP** (°C)**:** 4.5
MW: 150.08 **BP** (°C)**:** 89.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.215E-03	6.326E-01	25	B349	2 0 2 0 2	

570. $C_6H_2F_4$
1,2,3,5-Tetrafluorobenzene
1,2,4,6-Tetrafluorobenzene
m-Tetrafluorobenzene
1,3,4,5-Tetrafluorobenzene
RN: 2367-82-0 **MP** (°C)**:** –48
MW: 150.08 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-03	7.431E-01	25	B349	2 0 2 0 2	

571. $C_6H_2F_4O$
2,3,5,6-Tetrafluorophenol
1,2,4,5-Tetrafluoro-3-hydroxybenzene
RN: 769-39-1 **MP** (°C)**:** 38
MW: 166.08 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-01	6.145E+01	25	P031	0 0 0 0 0	

572. $C_6H_3Br_2NO_2$
2,6-Dibromoquinone oxime
RN: **MP** (°C)**:**
MW: 280.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-04	2.388E-01	20	G066	1 0 0 0 1	

573. $C_6H_3Br_3$
1,2,4-Tribromobenzene
Tribromobenzene, 1,2,4-
RN: 615-54-3 **MP** (°C)**:** 43
MW: 314.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E-05	3.670E-03	10	K440	0 0 0 0 0	
2.290E-05	7.210E-03	25	K440	0 0 0 0 0	
3.494E-05	1.100E-02	35	K440	0 0 0 0 0	

574. $C_6H_3Br_3O$
2,4,6-Tribromobiphenyl
1,1′-Biphenyl, 2,4,6-tribromo-
RN: 59080-33-0 **MP** (°C)**:** 66
MW: 330.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.111E-02	1.360E+01	26.5	G312	0 0 0 0 0	

575. $C_6H_3Br_3O$
2,4,6-Tribromophenol
2,4,6-Tribrom-phenol
Tribromophenol
Bromol
RN: 118-79-6 **MP** (°C)**:** 95
MW: 330.82 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.116E-04	7.000E-02	15	F300	1 0 0 0 1	
2.300E-04	7.609E-02	ns	O310	0 0 0 0 1	

576. $C_6H_3ClN_2O_4$
1-Chloro-2,4-dinitrobenzene
2,4-Dinitro-1-chlorobenzene
4-Chlor-1,3-dinitrobenzol
4-Chloro-1,3-dinitrobenzene
RN: 97-00-7 **MP** (°C)**:** 53
MW: 202.55 **BP** (°C)**:** 315

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-05	8.000E-03	15	D071	1 2 0 0 0	
3.950E-05	8.000E-03	15	F300	1 0 0 0 0	
4.560E-05	9.236E-03	25	G090	2 2 1 1 1	
2.023E-03	4.098E-01	50	D071	1 2 0 0 1	
7.837E-03	1.587E+00	100	D071	1 2 0 0 2	
8.393E-03	1.700E+00	100	F300	1 0 0 0 1	
7.244E-04	1.467E-01	ns	R427	0 0 0 0 0	

577. $C_6H_3ClN_4$
7-Chloropteridine
Pteridine, 7-chloro-
RN: 1125-84-4 **MP** (°C)**:** 95
MW: 166.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-01	2.174E+01	20	A083	1 2 0 0 0	

578. $C_6H_3Cl_2NO_2$
3,4-Dichloronitrobenzene
1,2-Dichloro-4-nitrobenzene
RN: 99-54-7 **MP** (°C)**:** 41.25
MW: 192.00 **BP** (°C)**:** 255.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.290E-04	1.208E-01	20	E308	1 2 2 1 2	

579. $C_6H_3Cl_2NO_2$
2,5-Dichloronitrobenzene
1,4-Dichloro-2-nitrobenzene
RN: 89-61-2 **MP** (°C)**:** 55.5
MW: 192.00 **BP** (°C)**:** 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	9.216E-02	20	E308	1 2 2 1 2	

580. $C_6H_3Cl_2NO_2$
2,3-Dichloronitrobenzene
1,2-Dichloro-3-nitrobenzene
RN: 3209-22-1 **MP** (°C)**:** 61.5
MW: 192.00 **BP** (°C)**:** 257.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-04	6.240E-02	20	E308	1 2 2 1 2	

581. $C_6H_3Cl_2NO_2$
3,6-Dichloropicolinic acid
3,6-Dichloro-2-pyridinecarboxylic acid
Clopyralid
Lontrel
Stinger
RN: 1702-17-6 **MP** (°C)**:** 151.5
MW: 192.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.208E-03	1.000E+00	20	M161	1 0 0 0 0	
5.208E-03	1.000E+00	ns	K138	0 0 0 0 1	

582. $C_6H_3Cl_3$
1,2,3-Trichlorobenzene
Benzene, 1,2,3-trichloro-
vic-Trichlorobenzene
RN: 87-61-6 **MP** (°C)**:** 51
MW: 181.45 **BP** (°C)**:** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-05	1.408E-02	20	K337	1 0 0 0 2	
6.607E-05	1.199E-02	22	K305	1 0 1 1 2	
8.983E-05	1.630E-02	23	C305	1 1 2 2 2	
9.920E-05	1.800E-02	25	B304	2 0 2 2 2	
1.170E-04	2.123E-02	25	B317	0 0 0 0 0	
9.920E-05	1.800E-02	25	C313	0 0 0 0 0	
6.760E-05	1.227E-02	25	M342	1 0 1 1 2	
9.149E-05	1.660E-02	ns	H123	0 0 0 0 0	
6.760E-05	1.227E-02	ns	M308	0 0 1 1 2	

583. $C_6H_3Cl_3$
1,3,5-Trichlorobenzene
Benzene, 1,3,5-trichloro-
RN: 108-70-3 **MP** (°C)**:** 64
MW: 181.45 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-05	4.353E-03	20	K337	1 0 0 0 2	
3.236E-05	5.872E-03	22	K305	1 0 1 1 2	
5.842E-05	1.060E-02	23	C305	1 1 2 2 2	
3.312E-05	6.010E-03	25	B304	2 0 2 2 2	
2.900E-05	5.262E-03	25	B317	0 0 0 0 0	
2.270E-05	4.119E-03	25	M342	1 0 1 1 2	
2.270E-05	4.119E-03	ns	M308	0 0 1 1 2	

584. $C_6H_3Cl_3$
1,2,4-Trichlorobenzene
Benzene, 1,2,4-trichloro-
RN: 120-82-1 **MP** (°C)**:** 17
MW: 181.45 **BP** (°C)**:** 213

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	3.000E-02	19	M172	1 0 0 0 0	
1.950E-04	3.538E-02	20	K337	1 0 0 0 2	
1.072E-04	1.944E-02	22	K305	1 0 1 1 2	
1.725E-04	3.130E-02	25	B304	2 0 2 2 2	
2.200E-04	3.992E-02	25	B317	0 0 0 0 0	
2.692E-04	4.884E-02	25	C113	1 0 2 2 2	
2.540E-04	4.609E-02	25	M342	1 0 1 1 2	
3.555E-04	6.451E-02	30	M300	1 1 2 2 2	
3.555E-04	6.450E-02	30	M311	1 1 2 2 2	
2.540E-04	4.609E-02	ns	M308	0 0 1 1 2	

585. $C_6H_3Cl_3N_2O_2$
Picloram
4-Amino-3,5,6-trichloropicolinic acid
RN: 1918-02-1 **MP** (°C)**:** 241
MW: 241.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.967E-03	4.750E-01	10	C031	2 0 2 2 2	pH 2.8
2.260E-03	5.457E-01	20	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	25	B185	0 0 0 0 0	
1.781E-03	4.300E-01	25	B200	1 0 0 0 1	
1.781E-03	4.300E-01	25	M161	1 0 0 0 2	
2.830E-03	6.833E-01	30	C031	2 0 2 2 2	pH 2.8
3.290E-03	7.944E-01	40	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	ns	K138	0 0 0 0 1	
1.780E-03	4.298E-01	ns	M061	0 0 0 0 1	
3.500E-04	8.451E-02	ns	O025	2 2 2 2 1	intrinsic

586. $C_6H_3Cl_3O$
2,3,4-Trichlorophenol
2,3,4-Trichlorphenol
RN: 15950-66-0 **MP** (°C)**:** 80
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-03	9.150E-01	25	M373	1 0 2 1 2	
2.138E-03	4.221E-01	ns	R424	0 0 0 0 0	

587. $C_6H_3Cl_3O$
2,3,5-Trichlorophenol
2,3,5-Trichlorphenol
RN: 933-78-8 **MP** (°C)**:** 62
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.905E-03	7.710E-01	25	M373	1 0 2 1 2	

588. $C_6H_3Cl_3O$
2,3,6-Trichlorophenol
2,3,6-Trichlorphenol
RN: 933-75-5 **MP** (°C)**:** 58
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.993E-03	5.910E-01	25	M373	1 0 2 1 2	

589. $C_6H_3Cl_3O$
2,4,6-Trichlorophenol
2,4,6-Trichlorphenol
Dowicide 25
RN: 88-06-2 **MP** (°C)**:** 69
MW: 197.45 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-03	5.000E-01	11.20	F300	1 0 0 0 0	
2.076E-03	4.100E-01	19.5	A400	2 1 2 2 2	
2.163E-03	4.270E-01	20.1	A400	2 1 2 2 2	
4.558E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.505E-03	6.920E-01	24.9	A400	2 1 2 2 2	
2.200E-03	4.344E-01	25	B316	0 0 0 0 0	
3.586E-03	7.080E-01	25	M373	1 0 2 1 2	
4.554E-03	8.992E-01	25	R041	0 0 0 0 0	
4.558E-03	9.000E-01	25.40	F300	1 0 0 0 0	

(*continued*)

589. $C_6H_3Cl_3O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.077E-02	6.075E+00	29.8	A400	2 1 2 2 2	
3.292E-02	6.501E+00	35.1	A400	2 1 2 2 2	
1.266E-02	2.500E+00	96	F300	1 0 0 0 1	
<5.06E-03	<9.99E-01	ns	N034	0 0 0 0 0	
3.981E-03	7.861E-01	ns	R427	0 0 0 0 0	

590. $C_6H_3Cl_3O$
2,4,5-Trichloro-phenol
Phenol, 2,4,5-trichloro-
Dowicide 2
Preventol I
2,4,5-Trichlorophenol
Collunosol
RN: 95-95-4 **MP** (°C)**:** 69
MW: 197.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-03	9.478E-01	25	B316	0 0 0 0 0	
3.287E-03	6.490E-01	25	M373	1 0 2 1 2	

591. $C_6H_3Cl_4N$
Nitrapyrin
2-Chloro-6-(trichloromethyl)pyridine
Donco-163
N-Serve(R)
RN: 1929-82-4 **MP** (°C)**:** 62.5
MW: 230.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.738E-04	4.013E-02	20	B179	0 0 0 0 0	
1.732E-04	4.000E-02	20	G079	1 1 0 0 2	
3.118E-04	7.200E-02	ns	V414	0 0 0 0 0	

592. $C_6H_3FN_2O_4$
1-Fluoro-2,4-dinitrobenzene
FDNB
RN: 70-34-8 **MP** (°C)**:** 26
MW: 186.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.149E-03	4.000E-01	ns	B160	0 0 0 0 2	

593. $C_6H_3F_3O$
Trifluorophenol
2,3,4-Trifluorophenol
RN: 2822-41-5 **MP** (°C)**:**
MW: 148.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	6.220E+01	25	P031	0 0 0 0 0	

594. $C_6H_3N_3O_6$
sym-Trinitrobenzene
1,3,5-Trinitro-benzol
1,3,5-Trinitrobenzene
RN: 99-35-4 **MP** (°C)**:** 122.5
MW: 213.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	2.780E-01	15	D066	1 2 0 0 2	
1.304E-03	2.779E-01	15	D070	1 2 0 0 2	
1.314E-03	2.800E-01	15	F300	1 0 0 0 1	
1.678E-03	3.577E-01	25	H434	0 0 0 0 0	
4.786E-03	1.020E+00	50	D066	1 2 0 0 2	
4.781E-03	1.019E+00	50	D070	1 2 0 0 2	
2.337E-02	4.980E+00	100	D066	1 2 0 0 2	
2.325E-02	4.955E+00	100	D070	1 2 0 0 2	
2.393E-02	5.100E+00	100	F300	1 0 0 0 1	
1.288E-03	2.745E-01	ns	R427	0 0 0 0 0	

595. $C_6H_3N_3O_7$
Picric acid
2,4,6-Trinitrophenol
Picronitric acid
Pikrinsaeure
RN: 88-89-1 **MP** (°C)**:** 122.5
MW: 229.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.948E-02	6.754E+00	0	D077	1 0 0 1 1	
4.322E-02	9.901E+00	0	M043	1 0 0 0 1	
4.364E-02	9.999E+00	7.10	E032	1 2 1 2 2	
4.232E-02	9.695E+00	9	D080	1 2 0 0 2	unit assumed
3.507E-02	8.035E+00	10	D077	1 0 0 1 1	
4.749E-02	1.088E+01	10	M043	1 0 0 0 1	
4.407E-02	1.010E+01	18.90	E032	1 2 1 2 2	
4.792E-02	1.098E+01	20	D077	1 0 0 1 2	
5.151E-02	1.180E+01	20	H048	1 0 0 0 2	unit assumed
4.300E-02	9.852E+00	20	K310	1 0 0 1 1	

(*continued*)

595. $C_6H_3N_3O_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-02	1.186E+01	20	M043	1 0 0 0 1	
4.932E-02	1.130E+01	23.50	F300	0 0 0 0 2	
5.327E-02	1.220E+01	25	D058	1 0 1 1 2	
5.520E-02	1.265E+01	25	F030	1 0 2 1 2	
5.684E-02	1.302E+01	25	H048	1 0 0 0 2	unit assumed
5.780E-02	1.324E+01	25	K040	1 0 2 1 2	
5.474E-02	1.254E+01	25	M094	1 0 0 1 2	
6.026E-02	1.381E+01	30	D077	1 0 0 1 2	
6.450E-02	1.478E+01	30	M043	1 0 0 0 1	
7.465E-02	1.710E+01	33.30	E032	1 2 1 2 2	
7.633E-02	1.749E+01	40	D077	1 0 0 1 2	
8.138E-02	1.865E+01	40	M043	1 0 0 0 1	
9.396E-02	2.153E+01	44.30	E032	1 2 1 2 2	
9.354E-02	2.143E+01	50	D077	1 0 0 1 2	
9.930E-02	2.275E+01	50	D080	1 2 0 0 2	unit assumed
1.193E-01	2.733E+01	60	D077	1 0 0 1 2	
1.312E-01	3.007E+01	60	M043	1 0 0 0 1	
1.398E-01	3.204E+01	62.90	E032	1 2 1 2 2	
1.464E-01	3.354E+01	70	D077	1 0 0 1 2	
1.703E-01	3.902E+01	72.60	E032	1 2 1 2 2	
1.844E-01	4.224E+01	80	D077	1 0 0 1 2	
1.920E-01	4.398E+01	80	M043	1 0 0 0 1	
1.956E-01	4.481E+01	82	D080	1 2 0 0 2	unit assumed
2.007E-01	4.598E+01	83.90	E032	1 2 1 2 2	
2.362E-01	5.411E+01	90	D077	1 0 0 1 2	
2.160E-01	4.949E+01	90	K310	1 0 0 1 2	
2.244E-01	5.141E+01	90.10	E032	1 2 1 2 2	
2.326E-01	5.330E+01	92.40	E032	1 2 1 2 2	
2.517E-01	5.767E+01	94.80	E032	1 2 1 2 2	
2.947E-01	6.751E+01	100	D077	1 0 0 1 2	
3.083E-01	7.063E+01	100	D080	1 2 0 0 2	unit assumed
3.055E-01	7.000E+01	100	F300	1 0 0 0 1	
2.932E-01	6.716E+01	100	M043	1 0 0 0 1	

596. $C_6H_3N_3O_8$

Styphnic acid
Styphninsaeure

RN: 82-71-3 **MP** (°C)**:** 176
MW: 245.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-02	5.865E+00	6.10	E032	1 2 1 2 2	
2.167E-02	5.312E+00	16.60	E032	1 2 1 2 2	
2.203E-02	5.400E+00	25	F300	1 0 0 0 1	
2.179E-02	5.341E+00	25	K040	1 0 2 1 2	
2.997E-02	7.346E+00	35.70	E032	1 2 1 2 2	
3.471E-02	8.507E+00	47.10	E032	1 2 1 2 2	

(*continued*)

596. $C_6H_3N_3O_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.119E-02	1.010E+01	56.90	E032	1 2 1 2 2	
4.692E-02	1.150E+01	62	F300	1 0 0 0 2	
4.758E-02	1.166E+01	63.00	E032	1 2 1 2 2	
6.109E-02	1.497E+01	71.20	E032	1 2 1 2 2	
7.135E-02	1.749E+01	76.20	E032	1 2 1 2 2	
8.000E-02	1.961E+01	80.30	E032	1 2 1 2 2	
9.562E-02	2.344E+01	85.00	E032	1 2 1 2 2	
1.096E-01	2.686E+01	89.80	E032	1 2 1 2 2	
1.357E-01	3.326E+01	95.90	E032	1 2 1 2 2	

597. C_6H_4BrF

1-Bromo-2-fluorobenzene
2-Bromofluorobenzene

RN: 1072-85-1 **MP** (°C)**:**
MW: 175.01 **BP** (°C)**:** 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.018E-03	3.532E-01	25	B349	2 0 2 0 2	

598. C_6H_4BrF

1-Bromo-3-fluorobenzene
3-Bromofluorobenzene

RN: 1073-06-9 **MP** (°C)**:**
MW: 175.01 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.162E-03	3.784E-01	25	B349	2 0 2 0 2	

599. $C_6H_4BrNO_3$

2-Bromo-4-nitrophenol
2-Brom-4-nitro-phenol

RN: 5847-59-6 **MP** (°C)**:** 114
MW: 218.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	2.200E+01	100	F300	1 0 0 0 1	

600. $C_6H_4Br_2$
m-Dibromobenzene
1,3-Dibromobenzene
RN: 108-36-1 **MP** (°C)**:** –7
MW: 235.92 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-04	6.747E-02	35	H077	2 2 2 2 2	

601. $C_6H_4Br_2$
p-Dibromobenzene
1,4-Dibromobenzene
RN : 106-37-6 **MP** (°C)**:** 87.3
MW: 235.92 **BP** (°C)**:** 220.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-05	9.910E-03	10	K440	0 0 0 0 0	
8.478E-05	2.000E-02	25	A003	1 0 1 2 1	
5.900E-03	1.392E+00	25	C316	0 0 0 0 0	0.1M NaCl
7.206E-05	1.700E-02	25	K440	0 0 0 0 0	
1.120E-04	2.642E-02	35	H077	2 2 2 2 2	
1.043E-04	2.460E-02	35	K440	0 0 0 0 0	

602. C_6H_4ClF
1-Chloro-2-fluorobenzene
2-Chlorofluorobenzene
RN: 348-51-6 **MP** (°C)**:** –43
MW: 130.55 **BP** (°C)**:** 137.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-03	5.019E-01	25	B349	2 0 2 0 2	

603. C_6H_4ClF
1-Chloro-3-fluorobenzene
3-Chlorofluorobenzene
RN: 625-98-9 **MP** (°C)**:**
MW: 130.55 **BP** (°C)**:** 127.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.517E-03	5.897E-01	25	B349	2 0 2 0 2	

604. $C_6H_4ClIO_2S$

Pipsyl chloride
p-Iodobenzenesulfonyl chloride
RN: 98-61-3 **MP** (°C)**:** 81
MW: 302.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.388E-05	1.630E-02	25	B048	1 0 2 2 2	
8.793E-05	2.660E-02	35	B048	1 0 2 2 2	
1.646E-04	4.980E-02	50	B048	1 0 2 2 2	

605. $C_6H_4ClNO_2$

6-Chloropicolinic acid
Pyridinecarboxylic acid, 6-chloro-
RN: 4684-94-0 **MP** (°C)**:**
MW: 157.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.158E-02	3.400E+00	ns	K138	0 0 0 0 1	
2.138E-02	3.369E+00	ns	R427	0 0 0 0 0	

606. $C_6H_4ClNO_2$

p-Chloronitrobenzene
4-Nitrochlorobenzene
4-CNB
4-Chloronitrobenzene
RN: 100-00-5 **MP** (°C)**:** 82
MW: 157.56 **BP** (°C)**:** 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.711E-04	1.530E-01	9.99	B403	1 2 2 2 2	
1.777E-04	2.800E-02	17	D071	1 2 0 0 1	
1.777E-04	2.800E-02	17	F300	1 0 0 0 1	
1.327E-03	2.090E-01	19.99	B403	1 2 2 2 2	
2.877E-03	4.533E-01	20	E308	1 2 2 1 2	
1.429E-03	2.251E-01	20	H118	1 1 1 1 2	
1.429E-03	2.251E-01	20	H301	0 0 0 0 0	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.600E-03	2.521E-01	25	G090	2 2 1 1 1	
1.739E-03	2.740E-01	29.99	B403	1 2 2 2 2	
2.348E-03	3.700E-01	39.99	B403	1 2 2 2 2	
7.933E-04	1.250E-01	50	D071	1 2 0 0 2	
9.709E-04	1.530E-01	100	D071	1 2 0 0 2	
1.016E-03	1.600E-01	100	F300	1 0 0 0 2	

607. $C_6H_4ClNO_2$

m-Chloronitrobenzene
1-Chloro-3-nitrobenzene
3-Chloronitrobenzene
m-Nitrochlorobenzene

RN: 121-73-3 **MP** (°C)**:** 46.0
MW: 157.56 **BP** (°C)**:** 236.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.732E-03	2.729E-01	20	E308	1 2 2 1 2	

608. $C_6H_4ClNO_2$

o-Chloronitrobenzene
2-Nitrochlorobenzene
2-CNB
1-Chloro-2-nitrobenzene

RN: 88-73-3 **MP** (°C)**:** 32
MW: 157.56 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-03	2.280E-01	9.99	B403	1 2 2 2 2	
2.133E-03	3.360E-01	19.99	B403	1 2 2 2 2	
2.800E-03	4.412E-01	20	E308	1 2 2 1 2	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
3.470E-03	5.467E-01	25	G090	2 2 1 1 1	
3.199E-03	5.040E-01	29.99	B403	1 2 2 2 2	
4.271E-03	6.730E-01	39.99	B403	1 2 2 2 2	

609. $C_6H_4Cl_2$

1,2-Dichlorobenzene
o-Dichlorobenzene

RN: 95-50-1 **MP** (°C)**:** –17
MW: 147.00 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.047E-04	1.330E-01	3.5	C094	1 0 0 0 2	
1.007E-03	1.480E-01	20	C094	1 0 0 0 2	
9.114E-04	1.340E-01	20	K056	1 0 2 2 2	
9.550E-04	1.404E-01	20	K337	1 0 0 0 2	
6.607E-04	9.713E-02	22	K305	1 0 1 1 2	
<1.36E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.060E-03	1.558E-01	25	B173	2 0 2 2 2	
9.864E-04	1.450E-01	25	B185	0 0 0 0 0	
9.319E-04	1.370E-01	25	B304	2 0 2 2 2	
8.000E-04	1.176E-01	25	B317	0 0 0 0 0	
1.047E-03	1.539E-01	25	C113	1 0 2 2 2	
9.864E-04	1.450E-01	25	K056	1 0 2 2 2	
1.156E-03	1.700E-01	25	L319	1 0 2 1 1	
6.280E-04	9.232E-02	25	M342	1 0 1 1 2	
1.163E-03	1.710E-01	30	K056	1 0 2 2 2	

(*continued*)

609. $C_6H_4Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.016E-03	1.494E-01	30	M300	1 1 2 2 2	
9.680E-04	1.423E-01	30	M311	1 1 2 2 2	
1.245E-03	1.830E-01	35	K056	1 0 2 2 2	
1.320E-03	1.940E-01	40	K056	1 0 2 2 2	
1.381E-03	2.030E-01	45	K056	1 0 2 2 2	
1.517E-03	2.230E-01	55	K056	1 0 2 2 2	
1.578E-03	2.320E-01	60	K056	1 0 2 2 2	
1.060E+03	1.558E+05	ns	A096	0 0 0 0 2	*sic*
6.280E-04	9.232E-02	ns	M308	0 0 1 1 2	

610. $C_6H_4Cl_2$

1,3-Dichlorobenzene
m-Dichlorobenzene

RN: 541-73-1 **MP** (°C)**:** –24
MW: 147.00 **BP** (°C)**:** 172–173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-04	1.110E-01	20	K056	1 0 2 2 2	
7.943E-04	1.168E-01	20	K337	1 0 0 0 2	
4.677E-04	6.876E-02	22	K305	1 0 1 1 2	
9.080E-04	1.335E-01	25	B173	2 0 2 2 2	
9.728E-04	1.430E-01	25	B304	2 1 2 1 2	
8.300E-04	1.220E-01	25	B317	0 0 0 0 0	
9.120E-04	1.341E-01	25	C113	1 0 2 2 2	
8.367E-04	1.230E-01	25	K056	1 0 2 2 2	
8.470E-04	1.245E-01	25	M342	1 0 1 1 2	
9.523E-04	1.400E-01	30	K056	1 0 2 2 2	
8.537E-04	1.255E-01	30	M300	1 1 2 2 2	
8.537E-04	1.255E-01	30	M311	1 1 2 2 2	
1.020E-03	1.500E-01	35	K056	1 0 2 2 2	
1.136E-03	1.670E-01	40	K056	1 0 2 2 2	
1.204E-03	1.770E-01	45	K056	1 0 2 2 2	
1.333E-03	1.960E-01	55	K056	1 0 2 2 2	
1.367E-03	2.010E-01	60	K056	1 0 2 2 2	
9.080E+02	1.335E+05	ns	A096	0 0 0 0 2	*sic*
8.470E-04	1.245E-01	ns	M308	0 0 1 1 2	

611. $C_6H_4Cl_2$

1,4-Dichlorobenzene
p-Dichlorobenzene

RN: 106-46-7 **MP** (°C)**:** 53.1
MW: 147.00 **BP** (°C)**:** 173.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-04	6.880E-02	20	K056	1 2 2 1 2	average of 4
3.020E-04	4.439E-02	20	K337	1 0 0 0 2	
2.252E-04	3.310E-02	20	T301	1 2 2 2 2	

(*continued*)

611. $C_6H_4Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	4.868E-02	22	K305	1 0 1 1 2	
5.292E-04	7.780E-02	22.20	W003	2 2 2 2 2	average of 2
5.673E-04	8.340E-02	24.60	W003	2 2 2 2 2	average of 3
5.170E-04	7.600E-02	25	A003	1 0 1 2 1	
5.928E-04	8.715E-02	25	A058	1 1 1 1 2	
<3.40E-03	<5.00E-01	25	B019	1 0 1 2 0	
5.020E-04	7.380E-02	25	B173	2 0 2 2 2	
4.442E-04	6.530E-02	25	B304	2 0 2 2 2	
5.270E-04	7.747E-02	25	B317	0 0 0 0 0	
3.990E-04	5.865E-02	25	C316	0 0 0 0 0	0.1M NaCl
5.374E-04	7.900E-02	25	F071	1 1 2 1 1	
5.374E-04	7.900E-02	25	H080	1 0 0 0 1	
5.381E-04	7.910E-02	25	K056	1 2 2 2 2	average of 2
5.646E-04	8.300E-02	25	M040	1 0 0 1 1	
5.442E-04	8.000E-02	25	M161	1 0 0 0 1	
2.100E-04	3.087E-02	25	M342	1 0 1 1 2	
6.932E-05	1.019E-02	25	N311	1 0 1 1 2	
4.100E-04	6.027E-02	25.2	T428	0 0 0 0 0	
5.898E-04	8.670E-02	25.50	W003	2 2 2 2 2	average of 2
5.238E-04	7.699E-02	30	G029	1 0 2 2 1	
6.347E-04	9.330E-02	30	K056	1 2 2 2 2	
6.267E-04	9.213E-02	30	M300	1 1 2 2 2	
6.422E-04	9.440E-02	30	M311	1 1 2 2 2	
6.299E-04	9.260E-02	30.00	W003	2 2 2 2 2	average of 2
6.939E-04	1.020E-01	34.50	W003	2 2 2 2 2	average of 3
5.646E-04	8.300E-02	35	K056	1 2 2 2 2	
8.231E-04	1.210E-01	38.40	W003	2 2 2 2 2	
6.857E-04	1.008E-01	40	K056	1 2 2 2 2	average of 2
8.292E-04	1.219E-01	45	K056	1 2 2 2 2	average of 2
1.082E-03	1.590E-01	47.50	W003	2 2 2 2 2	
1.184E-03	1.740E-01	50.10	W003	2 2 2 2 2	average of 2
1.061E-03	1.560E-01	55	K056	1 2 2 2 2	
1.429E-03	2.100E-01	59.20	W003	2 2 2 2 2	
1.109E-03	1.630E-01	60	K056	1 2 2 2 2	
1.483E-03	2.180E-01	60.70	W003	2 2 2 2 2	average of 2
1.565E-03	2.300E-01	65.10	W003	2 2 2 2 2	average of 3
1.612E-03	2.370E-01	65.20	W003	2 2 2 2 2	average of 3
1.912E-03	2.810E-01	73.40	W003	2 2 2 2 2	
2.100E-04	3.087E-02	ns	M308	0 0 1 1 2	
5.374E-04	7.900E-02	ns	M344	0 0 0 0 1	
5.034E-04	7.400E-02	rt	S314	0 0 2 1 1	

612. $C_6H_4Cl_2N_2O_2$

Dicloran

RN: 99-30-9 **MP** (°C)**:** 195
MW: 207.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-05	6.252E-03	ns	R424	0 0 0 0 0	
3.020E-05	6.252E-03	ns	R427	0 0 0 0 0	

613. $C_6H_4Cl_2O$
2,4-Dichlorophenol
2,4-Dichlor-phenol
RN: 120-83-2 **MP** (°C)**:** 45
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.390E-02	3.896E+00	15.3	A400	2 1 2 2 2	
2.748E-02	4.480E+00	19	D041	1 0 0 0 1	
~2.76E-02	~4.50E+00	20	F300	1 0 0 0 0	
2.748E-02	4.480E+00	20	N034	1 0 0 0 1	
3.403E-02	5.547E+00	25	M373	1 0 2 1 2	
3.052E-02	4.975E+00	25	R041	0 0 0 0 0	
3.385E-02	5.517E+00	25.2	A400	2 1 2 2 2	
1.748E-01	2.850E+01	34.6	A400	2 1 2 2 2	
2.754E-02	4.490E+00	ns	R427	0 0 0 0 0	

614. $C_6H_4Cl_2O$
3,5-Dichlorophenol
3,5-DCP
RN: 591-35-5 **MP** (°C)**:** 68
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-02	7.394E+00	25	M373	1 0 2 1 2	

615. $C_6H_4Cl_2O$
3,4-Dichlorophenol
4,5-Dichlorophenol
3,4-DCP
RN: 95-77-2 **MP** (°C)**:** 67
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-02	9.256E+00	25	M373	1 0 2 1 2	

616. $C_6H_4Cl_2O$
2,6-Dichlorophenol
2,6-DCP
RN: 87-65-0 **MP** (°C)**:** 66.5
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-02	2.625E+00	25	M373	1 0 2 1 2	

617. $C_6H_4Cl_2O$
2,3-Dichlorophenol
Phenol, 2,3-dichloro-
RN: 576-24-9 **MP** (°C)**:** 59
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.040E-02	8.215E+00	25	M373	1 0 2 1 2	

618. $C_6H_4Cl_2O$
2,5-Dichlorophenol
2,5-Dichlor-phenol
RN: 583-78-8 **MP** (°C)**:**
MW: 163.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-02	6.194E+00	25	B316	0 0 0 0 0	

619. C_6H_4FI
1-Fluoro-4-iodobenzene
4-Fluoro-1-iodobenzene
p-Iodofluorobenzene
p-Fluoroiodobenzene
p-Fluorophenyl iodide
RN: 352-34-1 **MP** (°C)**:** –27
MW: 222.00 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-04	1.665E-01	25	B349	2 0 2 0 2	

620. $C_6H_4I_2$
1,4-Diiodobenzene
p-Diiodobenzene
4-Iodophenyl iodide
RN: 624-38-4 **MP** (°C)**:** 131
MW: 329.91 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.244E-06	1.400E-03	25	A003	1 2 1 2 1	*sic*
3.100E-02	1.023E+01	25	C316	0 0 0 0 0	0.1M NaCl

621. $C_6H_4N_2O_4$
p-Dinitrobenzene
1,4-Dinitrobenzene
RN: 100-25-4 **MP** (°C)**:** 173
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.759E-04	8.000E-02	20	F300	1 0 0 0 0	
2.350E-04	3.951E-02	25	C316	0 0 0 0 0	0.1M NaCl
4.090E-04	6.876E-02	25	I334	2 2 2 1 2	
3.676E-04	6.180E-02	25	L008	2 2 2 1 2	average of 2
6.170E-04	1.037E-01	35	H077	2 2 2 2 2	
1.130E-02	1.900E+00	100	F300	1 0 0 0 1	

622. $C_6H_4N_2O_4$
m-Dinitrobenzene
1,3-Dinitrobenzene
RN: 99-65-0 **MP** (°C)**:** 89.5
MW: 168.11 **BP** (°C)**:** 301.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.045E-04	6.800E-02	13	D070	1 2 0 0 1	
4.164E-04	7.000E-02	13	F300	1 0 0 0 0	
3.420E-03	5.749E-01	25	I334	2 2 2 1 2	
3.169E-03	5.328E-01	25	L008	2 2 2 1 2	average of 2
5.116E-03	8.600E-01	25.04	V013	2 2 2 2 2	
3.867E-03	6.500E-01	30	F300	1 0 0 0 1	
3.888E-03	6.536E-01	30	G029	1 0 2 2 2	
4.670E-03	7.851E-01	35	H077	2 2 2 2 2	
2.789E-03	4.688E-01	50	D070	1 2 0 0 2	
1.134E-02	1.906E+00	100	D070	1 2 0 0 2	
1.547E-02	2.600E+00	100	F300	1 0 0 0 1	
2.973E-03	4.998E-01	rt	D021	0 0 1 1 0	

623. $C_6H_4N_2O_4$
o-Dinitrobenzene
1,2-Dinitrobenzene
RN: 528-29-0 **MP** (°C)**:** 118
MW: 168.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.328E-04	1.400E-01	20	F300	1 0 0 0 1	
7.910E-04	1.330E-01	25	I334	2 2 2 1 2	
7.418E-04	1.247E-01	25	L008	2 2 2 1 2	average of 3

624. $C_6H_4N_2O_5$
3,5-Dinitrophenol
Phenol, θ-dinitro-
RN: 586-11-8 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.288E-02	1.342E+01	51.6	S117	1 2 1 1 2	solid hydrate
2.373E+00	4.370E+02	54.1	S117	1 2 1 1 2	anhydrate
2.407E+00	4.431E+02	54.5	S117	1 2 1 1 2	anhydrate
2.442E+00	4.496E+02	55.5	S117	1 2 1 1 2	anhydrate
2.474E+00	4.555E+02	57.9	S117	1 2 1 1 2	anhydrate
2.516E+00	4.633E+02	61.9	S117	1 2 1 1 2	anhydrate
2.583E+00	4.756E+02	69.9	S117	1 2 1 1 2	anhydrate
2.617E+00	4.819E+02	81.3	S117	1 2 1 1 2	anhydrate
5.308E-01	9.772E+01	109.3	S117	1 0 1 1 2	
1.253E+00	2.307E+02	124.6	S117	1 0 1 1 2	

625. $C_6H_4N_2O_5$
2,6-Dinitrophenol
β-Dinitrophenol
RN: 573-56-8 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-03	3.149E-01	15	D080	1 2 0 0 2	unit assumed
1.629E-03	3.000E-01	15	F300	1 0 0 0 0	
2.805E-02	5.164E+00	50	D080	1 2 0 0 2	unit assumed
6.547E-02	1.205E+01	100	D080	1 2 0 0 2	unit assumed
6.518E-02	1.200E+01	100	F300	1 0 0 0 1	

626. $C_6H_4N_2O_5$
2,4-Dinitrophenol
α-Dinitrophenol
Aldifen
Fenoxyl carbon N
RN: 51-28-5 **MP** (°C)**:** 107.5
MW: 184.11 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.097E-03	2.020E-01	12.5	D069	1 2 0 0 2	
1.086E-03	2.000E-01	12.50	F300	1 0 0 0 0	
1.629E-03	2.999E-01	15	D079	1 2 0 0 1	
2.254E-03	4.150E-01	15.1	A400	2 1 2 2 2	
3.025E-02	5.569E+00	18	D041	1 0 0 0 1	
2.800E-02	5.155E+00	20	K301	2 2 1 1 1	
2.524E-03	4.647E-01	25	H085	2 0 2 1 2	

(*continued*)

626. $C_6H_4N_2O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.467E-03	2.700E-01	25	P037	2 0 1 1 2	
3.753E-03	6.910E-01	25.0	A400	2 1 2 2 2	
1.901E-01	3.500E+01	35.0	A400	2 1 2 2 2	
4.356E-03	8.020E-01	50	D069	1 2 0 0 2	
9.504E-04	1.750E-01	50	D079	1 2 0 0 2	
7.431E-03	1.368E+00	54.50	E032	1 2 1 2 2	
1.192E-02	2.195E+00	67.60	E032	1 2 1 2 2	
1.630E-02	3.001E+00	75.80	E032	1 2 1 2 2	
3.414E-02	6.286E+00	85	D069	1 2 0 0 2	
3.170E-02	5.836E+00	87.40	E032	1 2 1 2 2	
4.845E-02	8.920E+00	92.40	E032	1 2 1 2 2	
6.547E-02	1.205E+01	96.20	E032	1 2 1 2 2	
7.163E-02	1.319E+01	100	D069	1 2 0 0 2	
8.964E-02	1.650E+01	100	D079	1 2 0 0 2	
7.061E-02	1.300E+01	100	F300	1 0 0 0 1	
2.444E-01	4.500E+01	h	F300	0 0 0 0 1	
2.702E-02	4.975E+00	ns	M061	0 0 0 0 0	

627. $C_6H_4N_2O_6$

2,4-Dinitroresorcinol
2,4-Dinitro-1,3-benzenediol

RN: 519-44-8 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-02	6.261E+00	57.70	E032	1 2 1 2 2	
4.801E-02	9.607E+00	66.60	E032	1 2 1 2 2	
7.434E-02	1.488E+01	69.50	E032	1 2 1 2 2	
9.895E-02	1.980E+01	76.50	E032	1 2 1 2 2	
1.690E-01	3.382E+01	84.70	E032	1 2 1 2 2	
2.380E-01	4.762E+01	90.00	E032	1 2 1 2 2	
3.495E-01	6.994E+01	93.00	E032	1 2 1 2 2	

628. $C_6H_4N_2O_6$

4,6-Dinitroresorcinol
4,6-Dinitro-1,3-benzenediol

RN: 616-74-0 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	3.998E-01	77.00	E032	1 2 1 2 2	
3.995E-03	7.994E-01	90.50	E032	1 2 1 2 2	
4.992E-03	9.990E-01	96.30	E032	1 2 1 2 2	

629. $C_6H_4N_4$
Pteridine
1,3,5,8-Tetraazanaphthalene
Azinepurine
Pyrimido[4,5-b]pyrazine
Pyrazino[2,3-d]pyrimidine
RN: 91-18-9 **MP** (°C)**:** 138
MW: 132.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.461E-01	1.250E+02	20	A020	1 2 0 0 1	
9.461E-01	1.250E+02	20	B050	1 0 0 0 0	
9.230E-01	1.220E+02	22.5	A085	1 2 0 0 0	
3.784E+00	5.000E+02	100	B050	1 0 0 0 0	

630. $C_6H_4N_4O$
4-Hydroxypteridine
4-Pteridinol
RN: 700-47-0 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-02	4.975E+00	20	A020	1 2 0 0 1	
3.359E-02	4.975E+00	20	B050	1 0 0 0 0	
3.359E-02	4.975E+00	22.5	A085	1 2 0 0 0	
2.250E-01	3.333E+01	100	B050	1 0 0 0 0	

631. $C_6H_4N_4O$
6-Hydroxypteridine
6-Pteridinol
RN: 2432-26-0 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-03	2.856E-01	20	A020	1 2 0 0 1	
1.928E-03	2.856E-01	20	B050	1 0 0 0 0	
2.923E-02	4.329E+00	100	B050	1 0 0 0 0	

632. $C_6H_4N_4O$
7-Hydroxypteridine
7-Pteridinol
RN: 2432-27-1 **MP** (°C)**:**
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.493E-03	1.110E+00	20	B050	1 0 0 0 0	
8.768E-02	1.299E+01	100	B050	1 0 0 0 0	

633. $C_6H_4N_4O$
2-Hydroxypteridine
2-Pteridinol
RN: 25911-76-6 **MP** (°C)**:** 240
MW: 148.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.664E+00	20	A020	1 2 0 0 1	
1.123E-02	1.664E+00	20	B050	1 0 0 0 0	
1.123E-02	1.664E+00	22.5	A085	1 2 0 0 0	
1.324E-01	1.961E+01	100	B050	1 0 0 0 0	

634. $C_6H_4N_4O_2$
2,4-Dihydroxypteridine
2:4-Dihydroxypteridine
Lumazine
RN: 487-21-8 **MP** (°C)**:** 348.5
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.607E-03	1.248E+00	20	B050	1 0 0 0 0	
7.607E-03	1.248E+00	22.5	A085	1 2 0 0 0	
5.035E-02	8.264E+00	100	B050	1 0 0 0 0	

635. $C_6H_4N_4O_2$
2,7-Dihydroxypteridine
2:7-Dihydroxypteridine
RN: 65882-62-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.033E-02	9.901E+00	100	A020	1 2 0 0 0	

636. $C_6H_4N_4O_2$
4,6-Dihydroxypteridine
4:6-Dihydroxypteridine
RN: 16310-36-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.108E-03	1.818E-01	20	A020	1 2 0 0 1	
1.218E-03	2.000E-01	20	B050	1 0 0 0 0	
2.024E-02	3.322E+00	100	B050	1 0 0 0 0	

637. $C_6H_4N_4O_2$
4,7-Dihydroxypteridine
4:7-Dihydroxypteridine
6,7-Dihydroxypteridine
6:7-Dihydroxypteridine
RN: 33669-70-4 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	3.332E-01	20	A020	1 2 0 0 1	
1.523E-03	2.499E-01	20	A020	1 2 0 0 1	
2.030E-03	3.332E-01	20	B050	1 0 0 0 0	
1.523E-03	2.499E-01	20	B050	1 0 0 0 0	
2.094E-02	3.436E+00	100	B050	1 0 0 0 0	
1.014E-02	1.664E+00	100	B050	1 0 0 0 0	

638. $C_6H_4N_4O_2$
2,6-Dihydroxypteridine
2:6-Dihydroxypteridine
RN: 89324-38-9 **MP** (°C)**:**
MW: 164.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.222E-01	100	A020	1 2 0 0 1	

639. $C_6H_4N_4O_3$
2,4,7-Trihydroxypteridine
2:4:7-Trihydroxypteridine
RN: 2577-38-0 **MP** (°C)**:**
MW: 180.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.626E-04	8.333E-02	20	A020	1 2 0 1 1	
4.626E-04	8.333E-02	20	B050	1 0 0 0 0	
3.963E-03	7.138E-01	100	A020	1 2 0 0 1	
3.963E-03	7.138E-01	100	B050	1 0 0 0 0	

640. $C_6H_4N_4O_3$
4,6,7-Trihydroxypteridine
4:6:7-Trihydroxypteridine
RN: 58947-88-9 **MP** (°C)**:**
MW: 180.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-04	3.704E-02	20	A020	1 2 0 0 1	
2.056E-04	3.704E-02	20	B050	1 0 0 0 0	
7.930E-04	1.428E-01	100	B050	1 0 0 0 0	

641. $C_6H_4N_4O_4$
2,4,6,7-Tetrahydroxypteridine
2,4,6-Trihydroxypteridine
2:4:6-Trihydroxypteridine
RN: 2817-14-3 **MP** (°C)**:**
MW: 196.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.791E-05	1.724E-02	20	A020	1 2 0 1 1	
6.889E-04	1.351E-01	20	B050	1 0 0 0 0	
8.791E-05	1.724E-02	20	B050	1 0 0 0 0	
1.272E-02	2.494E+00	100	A020	1 2 0 0 0	
7.283E-04	1.428E-01	100	A020	1 2 0 0 0	
1.272E-02	2.494E+00	100	B050	1 0 0 0 0	

642. $C_6H_4N_4O_6$
Picramine
2,4,6-Trinitroaniline
1-Amino-2,4,6-trinitrobenzene
MATB
RN: 489-98-5 **MP** (°C)**:** 192
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-05	1.987E-02	25	B335	1 2 0 0 1	

643. $C_6H_4N_4S$
4-Mercaptopteridine
4-Pteridinethiol
4(1H)-Pteridinethione
Pteridine-4-thiol
RN: 65882-61-3 **MP** (°C)**:** 176dec
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.691E-03	2.777E-01	22.5	A085	1 2 0 0 0	

644. $C_6H_4N_4S$
2-Mercaptopteridine
2-Pteridinethiol
2(1H)-Pteridinethione
RN: 16878-76-5 **MP** (°C)**:** 205
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.347E-03	7.138E-01	22.5	A085	1 2 0 0 0	

645. $C_6H_4N_4S$
7-Mercaptopteridine
7-Pteridinethiol
7(1H)-Pteridinethione
RN: 36653-71-1 **MP** (°C)**:**
MW: 164.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-03	3.225E-01	20	A083	1 2 0 0 0	
6.760E-03	1.110E+00	100	A083	1 2 0 0 0	

646. $C_6H_4O_2$
Quinone
1,4-Benzoquinone
Benzochinhydrone
p-Quinone
RN: 106-51-4 **MP** (°C)**:** 115.7
MW: 108.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-02	9.329E+00	11.85	L064	2 2 2 1 2	0.01N HCl
1.013E-01	1.095E+01	17.70	L065	1 0 0 0 2	0.01N HCl
1.021E-01	1.104E+01	17.90	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	17.95	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	18	L064	2 2 2 1 2	0.01N HCl
1.580E-02	1.708E+00	20	B113	1 2 2 1 2	
1.233E-01	1.333E+01	23.85	L064	2 2 2 1 2	0.01N HCl
1.295E-01	1.400E+01	24	F300	1 0 0 0 1	
1.266E-01	1.369E+01	25	G033	1 0 1 1 2	
1.397E-01	1.510E+01	25	K033	1 0 0 1 2	

647. $C_6H_4O_5$
2,5-Dicarboxyfuran
Furan-dicarbon-saeure-(2,5)
RN: 3238-40-2 **MP** (°C)**:**
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.406E-03	1.000E+00	18	F300	1 0 0 0 0	

648. $C_6H_4O_5$
2-Carboxy-5-hydroxy-4-pyrone
Komensaeure
Komenic acid
RN: 499-78-5 **MP** (°C)**:**
MW: 156.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.267E-02	5.100E+00	25	F300	1 0 0 0 1	
3.921E-01	6.120E+01	100	F300	1 0 0 0 2	

649. C_6H_5Br
Bromobenzene
Phenyl bromide
Monobromobenzene
RN: 108-86-1 **MP** (°C)**:** –30
MW: 157.02 **BP** (°C)**:** 156.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.611E-03	4.100E-01	25	A003	1 2 1 2 1	
2.620E-03	4.114E-01	25	W300	2 2 2 2 2	
2.840E-03	4.460E-01	30	F071	1 1 2 1 2	
2.966E-03	4.658E-01	30	G029	1 0 2 2 2	
2.840E-03	4.460E-01	30	H080	1 0 0 0 2	
2.102E-03	3.300E-01	30	M311	1 1 2 2 2	
2.799E-03	4.395E-01	30	V009	1 0 0 0 1	
2.920E-03	4.585E-01	35	H077	2 2 2 2 2	
5.110E-04	8.024E-02	ns	D348	0 0 0 0 0	
2.615E-03	4.106E-01	ns	M344	0 0 0 0 2	

650. C_6H_5BrO
p-Bromophenol
4-Bromophenol
RN: 106-41-2 **MP** (°C)**:** 66
MW: 173.02 **BP** (°C)**:** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.053E-02	1.393E+01	20	R087	0 0 0 0 0	0.15M NaCl
8.542E-02	1.478E+01	25	R041	0 0 0 0 0	
8.128E-02	1.406E+01	ns	R424	0 0 0 0 0	

651. $C_6H_5BrO_3S$

p-Bromobenzenesulfonic acid
4-Bromobenzenesulfonic acid
RN: 138-36-3 **MP** (°C)**:**
MW: 237.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E+00	4.929E+02	82.3	T023	1 2 2 1 2	
2.088E+00	4.949E+02	89.6	T023	1 2 2 1 2	
2.093E+00	4.961E+02	93.1	T023	1 2 2 1 2	
2.097E+00	4.972E+02	97.6	T023	1 2 2 1 2	

652. $C_6H_5BrO_3S.H_2O$

p-Bromobenzenesulfonic acid (monohydrate)
RN: 138-36-3 **MP** (°C)**:**
MW: 255.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E+00	4.588E+02	43.8	T023	1 2 2 1 2	
1.821E+00	4.644E+02	60.2	T023	1 2 2 1 2	
1.586E+00	4.045E+02	71.2	T023	1 2 2 1 2	
1.924E+00	4.909E+02	76.6	T023	1 2 2 1 2	
1.922E+00	4.903E+02	78.5	T023	1 2 2 1 2	
1.855E+00	4.731E+02	80.3	T023	1 2 2 1 2	
1.868E+00	4.766E+02	86.2	T023	1 2 2 1 2	
1.907E+00	4.865E+02	87.2	T023	1 2 2 1 2	
1.889E+00	4.818E+02	90.2	T023	1 2 2 1 2	

653. $C_6H_5BrO_3S.2.5H_2O$

p-Bromobenzenesulfonic acid (2.5 hydrate)
RN: 138-36-3 **MP** (°C)**:**
MW: 282.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.375E+00	3.880E+02	–21.0	T023	1 2 2 1 2	
1.409E+00	3.975E+02	–10.5	T023	1 2 2 1 2	
1.495E+00	4.219E+02	12.5	T023	1 2 2 1 2	
1.522E+00	4.294E+02	19.9	T023	1 2 2 1 2	
1.566E+00	4.418E+02	27.6	T023	1 2 2 1 2	
1.613E+00	4.550E+02	34.6	T023	1 2 2 1 2	
1.447E+00	4.081E+02	.0	T023	1 2 2 1 2	

654. C_6H_5Cl

Chlorobenzene
IP Carrier T 40
Phenyl chloride
Tetrosin SP
Monochlorobenzene
MCB

RN: 108-90-7 **MP** (°C)**:** −45
MW: 112.56 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-03	4.802E-01	20	K337	1 0 0 0 2	
4.440E-03	4.998E-01	20	M312	1 0 0 0 2	
4.742E-03	5.337E-01	21	C024	2 1 1 2 2	
4.442E-03	5.000E-01	25	A003	1 2 1 2 1	
4.191E-03	4.717E-01	25	A058	1 1 1 1 2	
<1.78E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.460E-03	5.020E-01	25	B304	2 0 2 2 2	
4.300E-03	4.840E-01	25	B317	0 0 0 0 0	
3.108E-03	3.499E-01	25	L319	1 0 2 1 1	
2.620E-03	2.949E-01	25	M342	1 0 1 1 2	
3.540E-02	3.984E+00	25	N309	1 0 0 0 1	*sic*
3.780E-03	4.255E-01	25	S359	2 1 2 2 2	
4.430E-03	4.986E-01	25	W300	2 2 2 2 2	
9.762E-03	1.099E+00	25.50	O005	2 0 2 2 1	*sic*
8.884E-04	1.000E-01	26.70	L095	2 2 1 1 2	
3.980E-03	4.480E-01	30	F071	1 1 2 1 2	
4.353E-03	4.900E-01	30	F300	1 0 0 0 1	
4.333E-03	4.878E-01	30	G029	1 0 2 2 2	
3.980E-03	4.480E-01	30	H080	1 0 0 0 2	
4.000E-03	4.502E-01	30	H332	2 2 2 2 0	
4.351E-03	4.898E-01	30	K065	2 0 2 1 2	
4.211E-03	4.740E-01	30	M300	1 1 2 2 2	
4.211E-03	4.740E-01	30	M311	1 1 2 2 2	
4.298E-03	4.838E-01	30	V009	1 0 0 0 1	
6.259E-03	7.045E-01	40	K065	2 0 2 1 2	
3.560E-03	4.007E-01	45	N043	1 0 2 2 2	
8.521E-03	9.591E-01	50	K065	2 0 2 1 2	
9.762E-03	1.099E+00	60	K065	2 0 2 1 2	
1.424E-02	1.602E+00	70	K065	2 0 2 1 2	
1.601E-02	1.802E+00	80	K065	2 0 2 1 2	
2.216E-02	2.494E+00	90	K065	2 0 2 1 2	
4.185E-03	4.711E-01	ns	H123	0 0 0 0 0	
2.620E-03	2.949E-01	ns	M308	0 0 1 1 2	
4.193E-03	4.720E-01	ns	M344	0 0 0 0 2	

655. $C_6H_5ClN_2O_4S$

4-Chloro-3-nitro-benzenesulfonamide
Benzenesulfonamide, 4-chloro-3-nitro-
RN: 97-09-6 **MP** (°C)**:**
MW: 236.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-04	2.248E-01	15	K024	1 2 1 1 2	

656. C_6H_5ClO

m-Chlorophenol
3-Chlorophenol
Chlorophenate
3-Hydroxychlorobenzene
RN: 108-43-0 **MP** (°C)**:** 33
MW: 128.56 **BP** (°C)**:** 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-01	2.500E+01	20	F300	1 0 0 0 1	
1.919E-01	2.468E+01	20	N034	1 0 0 0 2	
1.726E-01	2.219E+01	25	M373	1 0 2 1 2	
1.995E-01	2.565E+01	ns	R427	0 0 0 0 0	

657. C_6H_5ClO

p-Chlorophenol
4-Chloro-phenol-
Parachlorophenol
4-Hydroxychlorobenze
4-Chlorophenol
4-Hydroxychlorobenzene
RN: 106-48-9 **MP** (°C)**:** 43.2
MW: 128.56 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.815E-01	2.334E+01	15.1	A400	2 1 2 2 2	
2.022E-01	2.600E+01	20	F300	1 0 0 0 1	
1.022E-01	1.314E+01	20	H301	0 0 0 0 0	
1.993E-01	2.563E+01	20	N034	1 0 0 0 2	
1.839E-01	2.364E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.100E-01	2.700E+01	25	B316	0 0 0 0 0	
2.053E-01	2.639E+01	25	M373	1 0 2 1 2	
1.823E-01	2.344E+01	25	R041	0 0 0 0 0	
1.987E-01	2.554E+01	25.2	A400	2 1 2 2 2	
1.867E-01	2.401E+01	34.5	A400	2 1 2 2 2	
4.898E+00	6.297E+02	ns	R427	0 0 0 0 0	

658. C_6H_5ClO

o-Chlorophenol
2-Chlorophenol

RN: 95-57-8 **MP** (°C)**:** 9.3
MW: 128.56 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.621E-01	2.084E+01	15.4	A400	2 1 2 2 2	
1.763E-01	2.266E+01	24.6	A400	2 1 2 2 2	
8.830E-02	1.135E+01	25	B173	2 0 2 2 2	
1.809E-01	2.326E+01	25	M373	1 0 2 1 2	
1.674E-01	2.153E+01	25	R041	0 0 0 0 0	
2.097E-01	2.695E+01	ns	N034	0 0 0 0 2	

659. $C_6H_5ClO_3S$

p-Chlorobenzenesulfonic acid
4-Chlor-benzolsulfosaeure

RN: 98-66-8 **MP** (°C)**:** 67
MW: 192.62 **BP** (°C)**:** 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	4.975E+02	59.0	T023	1 2 2 1 2	
2.590E+00	4.988E+02	62.4	T023	1 2 2 1 2	

660. $C_6H_5ClO_3S.2.5H_2O$

p-Chlorobenzenesulfonic acid (2.5 hydrate)

RN: 98-66-8 **MP** (°C)**:**
MW: 237.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.519E+00	3.609E+02	–26.0	T023	1 2 2 1 2	
1.553E+00	3.690E+02	–20.0	T023	1 2 2 1 2	
1.606E+00	3.816E+02	–11.0	T023	1 2 2 1 2	
1.653E+00	3.929E+02	–2.2	T023	1 2 2 1 2	
1.723E+00	4.095E+02	10.6	T023	1 2 2 1 2	
1.784E+00	4.240E+02	22.9	T023	1 2 2 1 2	
1.817E+00	4.318E+02	27.6	T023	1 2 2 1 2	
1.854E+00	4.406E+02	30.8	T023	1 2 2 1 2	

661. $C_6H_5Cl_2NO_2S$

3,4-Dichloro-benzenesulfonamide
Benzenesulfonamide, 3,4-dichloro-

RN: 23815-28-3 **MP** (°C)**:**
MW: 226.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	7.913E-01	15	K024	1 2 1 1 2	

662. $C_6H_5Cl_2PS$
Dichlorophenylphosphine sulfide
Benzene phosphorus thiodichloride
Phenylphosphonothioic dichloride
Phenyl phosphorus thiodichloride
DCPPS
RN: 3497-00-5 **MP** (°C)**:**
MW: 211.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.211E-03	1.522E+00	23	W402	0 0 0 0 0	
2.597E-02	5.481E+00	32	W402	0 0 0 0 0	
4.676E-02	9.868E+00	40	W402	0 0 0 0 0	
7.060E-02	1.490E+01	50	W402	0 0 0 0 0	

663. C_6H_5F
Fluorobenzene
Fluorbenzol
RN: 462-06-6 **MP** (°C)**:** –42
MW: 96.11 **BP** (°C)**:** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	1.550E+00	25	A003	1 2 1 2 2	
1.602E-02	1.540E+00	30	F071	1 1 2 1 2	
1.561E-02	1.500E+00	30	F300	1 0 0 0 1	
1.602E-02	1.540E+00	30	H080	1 0 0 0 2	
1.600E-02	1.538E+00	30	J036	0 0 0 0 0	
1.598E-02	1.535E+00	30	V009	1 0 0 0 2	
1.616E-02	1.553E+00	ns	M344	0 0 0 0 2	

664. $C_6H_5FN_2O_3$
3-Acetyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Acetyl-5-fluorouracil
RN: 75410-15-0 **MP** (°C)**:** 115–116
MW: 172.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-01	4.280E+01	22	B321	0 0 0 0 0	pH 4.0
1.660E-01	2.857E+01	22	B416	2 2 1 2 1	

665. $C_6H_5FN_2O_4$
1-Methoxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, methyl ester
RN: 71759-43-8 **MP** (°C)**:**
MW: 188.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	2.330E+01	22	B332	1 1 0 0 1	pH 4.0

666. C_6H_5FO

2-Fluorophenol
2-Fluor-phenol
o-Fluorophenol

RN: 367-12-4 **MP** (°C)**:** 16.1
MW: 112.10 **BP** (°C)**:** 171.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

667. C_6H_5FO

m-Fluorophenol
3-Fluorophenol

RN: 372-20-3 **MP** (°C)**:** 13.7
MW: 112.10 **BP** (°C)**:** 178

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	7.735E+01	25	P031	0 0 0 0 0	

668. C_6H_5FO

p-Fluorophenol
4-Fluorophenol

RN: 371-41-5 **MP** (°C)**:** 46–48
MW: 112.10 **BP** (°C)**:** 185–188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.671E-01	6.357E+01	20	R087	0 0 0 0 0	0.15M NaCl
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

669. $C_6H_5FO_3S.H_2O$

p-Fluorobenzenesulfonic acid (monohydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 194.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E+00	4.355E+02	22.1	T023	1 2 2 1 2	
2.263E+00	4.394E+02	35.4	T023	1 2 2 1 2	
2.549E+00	4.950E+02	41.4	T023	1 2 2 1 2	
2.306E+00	4.477E+02	54.2	T023	1 2 2 1 2	
2.539E+00	4.930E+02	54.3	T023	1 2 2 1 2	
2.356E+00	4.575E+02	71.2	T023	1 2 2 1 2	
2.509E+00	4.872E+02	74.5	T023	1 2 2 1 2	
2.392E+00	4.644E+02	80.0	T023	1 2 2 1 2	
2.496E+00	4.847E+02	81.0	T023	1 2 2 1 2	
2.463E+00	4.782E+02	85.2	T023	1 2 2 1 2	
2.440E+00	4.739E+02	85.5	T023	1 2 2 1 2	

670. $C_6H_5FO_3S.2.5H_2O$

p-Fluorobenzenesulfonic acid (2.5 hydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 221.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.848E+00	4.088E+02	–15.5	T023	1 2 2 1 2	
1.880E+00	4.160E+02	–3.9	T023	1 2 2 1 2	
1.893E+00	4.187E+02	1.0	T023	1 2 2 1 2	
1.923E+00	4.254E+02	10.1	T023	1 2 2 1 2	
1.966E+00	4.349E+02	21.3	T023	1 2 2 1 2	

671. $C_6H_5FO_3S.3H_2O$

p-Fluorobenzenesulfonic acid (trihydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 230.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.731E+00	3.985E+02	–22.5	T023	1 2 2 1 2	
1.704E+00	3.922E+02	–21.4	T023	1 2 2 1 2	
1.751E+00	4.032E+02	–19.5	T023	1 2 2 1 2	
1.760E+00	4.052E+02	–17.9	T023	1 2 2 1 2	
1.715E+00	3.949E+02	–18.5	T023	1 2 2 1 2	
1.751E+00	4.032E+02	–13.0	T023	1 2 2 1 2	
1.784E+00	4.108E+02	–7.4	T023	1 2 2 1 2	

672. $C_6H_5FO_3S.4H_2O$

p-Fluorobenzenesulfonic acid (tetrahydrate)

RN: 368-88-7 **MP** (°C)**:**
MW: 248.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E+00	3.648E+02	–38.0	T023	1 2 2 1 2	
1.484E+00	3.684E+02	–35.4	T023	1 2 2 1 2	
1.498E+00	3.719E+02	–34.4	T023	1 2 2 1 2	
1.519E+00	3.771E+02	–32.5	T023	1 2 2 1 2	
1.532E+00	3.803E+02	–30.5	T023	1 2 2 1 2	
1.580E+00	3.922E+02	–26.4	T023	1 2 2 1 2	
1.605E+00	3.985E+02	–24.0	T023	1 2 2 1 2	

673. C_6H_5I

Iodobenzene

RN: 591-50-4 **MP** (°C)**:** –30
MW: 204.01 **BP** (°C)**:** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.823E-04	1.800E-01	25	A003	1 2 1 2 1	
9.840E-04	2.007E-01	25	M342	1 0 1 1 2	

(*continued*)

673. C_6H_5I (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-03	3.400E-01	30	F071	1 1 2 1 2	
1.667E-03	3.400E-01	30	F300	1 0 0 0 2	
1.667E-03	3.400E-01	30	H080	1 0 0 0 2	
1.667E-03	3.400E-01	30	M344	1 0 0 0 2	
1.699E-03	3.467E-01	30	V009	1 0 0 0 1	

674. C_6H_5IO

p-Iodophenol
4-Iodophenol

RN: 540-38-5 **MP** (°C)**:** 94
MW: 220.01 **BP** (°C)**:** 138 at 5 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-02	2.828E+00	20	R087	0 0 0 0 0	0.15M NaCl

675. $C_6H_5NO_2$

Nitrobenzene
Nitrobenzol
Benzene, nitro-

RN: 98-95-3 **MP** (°C)**:** 6
MW: 123.11 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	1.700E+00	6	V004	1 0 1 2 2	
1.438E-02	1.770E+00	9.99	B403	1 2 2 2 2	
1.443E-02	1.777E+00	15	G029	1 0 2 2 2	
1.568E-02	1.930E+00	19.99	B403	1 2 2 2 2	
1.549E-02	1.907E+00	20	B179	0 0 0 0 0	
1.543E-02	1.900E+00	20	F300	1 0 0 0 1	
1.600E-02	1.970E+00	20	P073	1 0 0 1 2	
1.543E-02	1.900E+00	22.5	G301	0 0 0 0 0	
1.568E-02	1.930E+00	25	A003	1 2 1 2 2	
1.700E-02	2.093E+00	25	B173	2 0 2 2 2	
1.580E-02	1.945E+00	25	H071	2 2 2 1 2	
1.600E-02	1.970E+00	25	H332	2 2 2 2 1	
1.560E-02	1.921E+00	25	I334	2 2 2 1 2	
1.560E-02	1.921E+00	25	I335	2 2 2 2 2	
1.543E-02	1.900E+00	25	M087	1 1 2 1 2	
1.457E-02	1.794E+00	25.04	V013	2 2 2 2 2	
1.446E-02	1.780E+00	26.70	L095	2 2 1 1 2	
1.673E-02	2.060E+00	29.99	B403	1 2 2 2 2	
1.662E-02	2.046E+00	30	G029	1 0 2 2 2	
1.673E-02	2.060E+00	30	V004	1 0 1 2 2	
1.667E-02	2.052E+00	30	V009	1 0 0 0 2	
1.835E-02	2.259E+00	35	H077	2 2 2 2 2	

(*continued*)

675. $C_6H_5NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-02	2.200E+00	39.99	B403	1 2 2 2 2	
2.144E-02	2.640E+00	50	V004	1 0 1 2 2	
2.193E-02	2.700E+00	55	F300	1 0 0 0 1	
2.534E-02	3.120E+00	60	V004	1 0 1 2 2	
2.700E-03	3.324E-01	ns	D348	0 0 0 0 0	

676. $C_6H_5NO_2$

Nicotinic acid
Niacin

RN: 59-67-6 **MP** (°C)**:** 236
MW: 123.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-01	1.488E+01	1	H083	1 2 2 1 2	
2.679E-01	3.298E+01	16	C033	1 0 2 1 2	
1.358E-01	1.672E+01	20	D041	1 0 0 0 1	
1.436E-01	1.768E+01	20	H083	1 2 2 1 2	
1.381E-01	1.700E+01	20	M054	1 0 0 0 1	
3.652E-01	4.496E+01	28	C033	1 0 2 1 2	
2.595E-01	3.195E+01	42	H083	1 2 2 1 2	
3.735E-01	4.598E+01	60	H083	1 2 2 1 2	
5.604E-01	6.899E+01	80	H083	1 2 2 1 2	
6.809E-01	8.383E+01	88	H083	1 2 2 1 2	

677. $C_6H_5NO_3$

o-Nitrophenol
2-Nitrophenol

RN: 88-75-5 **MP** (°C)**:** 44
MW: 139.11 **BP** (°C)**:** 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.434E-03	8.950E-01	9.99	B403	1 2 2 2 2	
7.735E-03	1.076E+00	15.6	A400	2 1 2 2 2	
9.704E-03	1.350E+00	19.99	B403	1 2 2 2 2	
1.000E-02	1.391E+00	20	H306	1 0 1 2 1	
9.906E-03	1.378E+00	23.10	E032	1 2 1 2 2	
1.220E-02	1.697E+00	24.8	A400	2 1 2 2 2	
1.793E-02	2.494E+00	25	D006	1 2 0 1 2	
1.797E-02	2.500E+00	25	D059	1 2 1 1 1	
1.438E-02	2.000E+00	29.99	B403	1 2 2 2 2	
1.163E-02	1.617E+00	30.40	E032	1 2 1 2 2	
2.110E-02	2.935E+00	34.7	A400	2 1 2 2 2	
1.456E-02	2.026E+00	36.20	E032	1 2 1 2 2	
2.300E-02	3.200E+00	38.40	F300	1 0 0 0 1	
1.936E-02	2.693E+00	39.80	E032	1 2 1 2 2	

(*continued*)

677. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.042E-02	2.840E+00	39.99	B403	1 2 2 2 2	
2.157E-02	3.000E+00	40	D059	1 2 1 1 0	
2.864E-02	3.984E+00	54.60	E032	1 2 1 2 1	
3.598E-02	5.005E+00	67.20	E032	1 2 1 2 2	
4.429E-02	6.162E+00	72.10	E032	1 2 1 2 2	
5.174E-02	7.198E+00	86.90	E032	1 2 1 2 2	
6.560E-02	9.126E+00	93.80	E032	1 2 1 2 2	
7.979E-02	1.110E+01	100	F300	1 0 0 0 2	

678. $C_6H_5NO_3$

p-Nitrophenol
4-Nitrophenol

RN: 100-02-7 **MP** (°C)**:** 113
MW: 139.11 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-02	4.975E+00	0	D006	1 2 0 1 1	
5.787E-02	8.050E+00	9.99	B403	1 2 2 2 2	
7.821E-02	1.088E+01	12.5	D006	1 2 0 1 1	
7.610E-02	1.059E+01	12.60	E032	1 2 1 2 2	
5.780E-02	8.040E+00	15	D069	1 2 0 0 2	
7.305E-02	1.016E+01	15.3	A400	2 1 2 2 2	
1.139E-01	1.584E+01	17.30	E032	1 2 1 2 2	
8.770E-02	1.220E+01	19.99	B403	1 2 2 2 2	
9.700E-02	1.349E+01	20	H306	1 0 1 2 1	
7.188E-02	9.999E+00	20	T301	1 2 2 2 2	
1.078E-01	1.500E+01	22.5	G301	0 0 0 0 0	
1.132E-01	1.575E+01	25	D006	1 2 0 1 1	
1.797E-01	2.500E+01	25	D059	1 2 1 1 1	
8.411E-02	1.170E+01	25	F300	1 0 0 0 2	
9.925E-02	1.381E+01	25	R041	0 0 0 0 0	
1.121E-01	1.560E+01	25.0	A400	2 1 2 2 2	
1.430E-01	1.990E+01	26.60	E032	1 2 1 2 2	
1.794E-01	2.496E+01	27.70	E032	1 2 1 2 2	
2.101E-01	2.922E+01	29.60	E032	1 2 1 2 2	
1.280E-01	1.780E+01	29.99	B403	1 2 2 2 2	
1.409E-01	1.960E+01	30.3	A400	2 1 2 2 2	
1.930E-01	2.685E+01	34.9	A400	2 1 2 2 2	
1.718E-01	2.390E+01	37.99	B403	1 2 2 2 2	
2.026E-01	2.818E+01	40	D006	1 2 0 1 1	
2.085E-01	2.900E+01	40	D059	1 2 1 1 1	
3.021E+00	4.203E+02	40.60	E032	1 2 1 2 2	
2.678E-01	3.726E+01	40.70	E032	1 2 1 2 2	
3.081E+00	4.286E+02	42.50	E032	1 2 1 2 2	
2.961E+00	4.120E+02	42.70	E032	1 2 1 2 2	
3.196E+00	4.447E+02	49.70	E032	1 2 1 2 2	
4.350E-01	6.052E+01	50	D069	1 2 0 0 2	
4.148E-01	5.770E+01	50	F300	1 0 0 0 2	

(*continued*)

678. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.096E-01	4.306E+01	53.30	E032	1 2 1 2 2	
2.900E+00	4.034E+02	54.90	E032	1 2 1 2 2	
3.423E-01	4.762E+01	55.10	E032	1 2 1 2 2	
3.305E+00	4.598E+02	60.70	E032	1 2 1 2 2	
2.834E+00	3.942E+02	65.00	E032	1 2 1 2 2	
3.986E-01	5.545E+01	67.80	E032	1 2 1 2 2	
5.021E-01	6.985E+01	69.40	E032	1 2 1 2 2	
2.768E+00	3.850E+02	73.30	E032	1 2 1 2 2	
3.406E+00	4.739E+02	75.70	E032	1 2 1 2 2	
6.553E-01	9.116E+01	78.30	E032	1 2 1 2 2	
6.837E-01	9.510E+01	79.80	E032	1 2 1 2 2	
2.699E+00	3.754E+02	80.30	E032	1 2 1 2 2	
7.124E-01	9.910E+01	80.70	E032	1 2 1 2 2	
7.987E-01	1.111E+02	82.30	E032	1 2 1 2 2	
9.431E-01	1.312E+02	85.70	E032	1 2 1 2 2	
2.555E+00	3.554E+02	86.00	E032	1 2 1 2 2	
1.076E+00	1.497E+02	88.50	E032	1 2 1 2 2	
2.398E+00	3.336E+02	89.70	E032	1 2 1 2 2	
1.320E+00	1.837E+02	90.70	E032	1 2 1 2 2	
1.438E+00	2.000E+02	91.30	E032	1 2 1 2 2	
2.234E+00	3.107E+02	91.30	E032	1 2 1 2 2	
1.664E+00	2.315E+02	92.10	E032	1 2 1 2 2	
2.056E+00	2.861E+02	92.70	E032	1 2 1 2 2	
1.763E+00	2.453E+02	92.80	E032	1 2 1 2 2	
1.865E+00	2.595E+02	92.90	E032	1 2 1 2 2	
3.503E+00	4.873E+02	93.50	E032	1 2 1 2 2	
5.100E-02	7.095E+00	ns	B157	0 0 0 0 1	
1.148E-01	1.597E+01	ns	R427	0 0 0 0 0	

679. $C_6H_5NO_3$

m-Nitrophenol
3-Nitrophenol

RN: 554-84-7 **MP** (°C)**:** 97
MW: 139.11 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.412E-02	8.920E+00	0	D006	1 2 0 1 1	
5.176E-02	7.200E+00	9.99	B403	1 2 2 2 2	
8.524E-02	1.186E+01	12.5	D006	1 2 0 1 1	
1.243E-01	1.730E+01	15.90	E032	1 2 1 2 2	
7.764E-02	1.080E+01	19.99	B403	1 2 2 2 2	
8.300E-02	1.155E+01	20	H306	1 0 1 2 1	
1.368E-01	1.903E+01	20.20	E032	1 2 1 2 2	
1.458E-01	2.028E+01	23.40	E032	1 2 1 2 2	
9.575E-02	1.332E+01	25	D006	1 2 0 1 2	
9.740E-02	1.355E+01	25	K040	1 0 2 1 2	
9.225E-02	1.283E+01	25	R041	0 0 0 0 0	

(*continued*)

679. $C_6H_5NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-01	2.344E+01	29.50	E032	1 2 1 2 2	
1.200E-01	1.670E+01	29.99	B403	1 2 2 2 2	
1.366E-01	1.900E+01	34.99	B403	1 2 2 2 2	
1.944E-01	2.705E+01	35.80	E032	1 2 1 2 2	
2.113E-01	2.940E+01	40	F300	1 0 0 0 2	
2.148E-01	2.988E+01	40.90	E032	1 2 1 2 2	
3.196E+00	4.445E+02	47.10	E032	1 2 1 2 2	
3.046E+00	4.237E+02	49.60	E032	1 2 1 2 2	
3.240E+00	4.507E+02	49.70	E032	1 2 1 2 2	
3.313E+00	4.609E+02	56.50	E032	1 2 1 2 2	
2.979E+00	4.145E+02	58.70	E032	1 2 1 2 2	
2.911E-01	4.049E+01	58.80	E032	1 2 1 2 2	
3.475E-01	4.834E+01	62.70	E032	1 2 1 2 2	
3.387E+00	4.712E+02	62.80	E032	1 2 1 2 2	
2.914E+00	4.054E+02	71.50	E032	1 2 1 2 2	
3.484E+00	4.846E+02	75.10	E032	1 2 1 2 2	
4.703E-01	6.542E+01	77.10	E032	1 2 1 2 2	
2.828E+00	3.935E+02	80.60	E032	1 2 1 2 2	
6.326E-01	8.801E+01	85.30	E032	1 2 1 2 2	
3.549E+00	4.937E+02	85.80	E032	1 2 1 2 2	
2.705E+00	3.762E+02	89.40	E032	1 2 1 2 2	
3.569E+00	4.965E+02	89.80	E032	1 2 1 2 2	
2.649E+00	3.684E+02	92.20	E032	1 2 1 2 2	
9.501E-01	1.322E+02	93.60	E032	1 2 1 2 2	
2.581E+00	3.591E+02	94.20	E032	1 2 1 2 2	
2.475E+00	3.443E+02	95.60	E032	1 2 1 2 2	
1.210E+00	1.683E+02	96.20	E032	1 2 1 2 2	
2.396E+00	3.333E+02	96.60	E032	1 2 1 2 2	
1.440E+00	2.004E+02	97.50	E032	1 2 1 2 2	
2.286E+00	3.181E+02	97.70	E032	1 2 1 2 2	
1.604E+00	2.232E+02	98.10	E032	1 2 1 2 2	
2.341E+00	3.256E+02	98.10	E032	1 2 1 2 2	
1.763E+00	2.453E+02	98.40	E032	1 2 1 2 2	
2.049E+00	2.851E+02	98.50	E032	1 2 1 2 2	
1.965E+00	2.734E+02	98.60	E032	1 2 1 2 2	
3.008E+00	4.184E+02	98.70	F300	1 0 0 0 2	
9.772E-02	1.359E+01	ns	R427	0 0 0 0 0	

680. $C_6H_5NO_4$

Nitrohydroquinone
2-Nitroquinol
4-Hydroxy-2-nitrophenol

RN: 16090-33-8 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.888E-02	1.068E+01	30.20	E032	1 2 1 2 2	
1.015E-01	1.575E+01	34.60	E032	1 2 1 2 2	

(*continued*)

680. $C_6H_5NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E-01	2.439E+01	44.60	E032	1 2 1 2 2	
1.999E-01	3.101E+01	49.60	E032	1 2 1 2 2	
3.128E-01	4.853E+01	54.50	E032	1 2 1 2 2	
4.498E-01	6.977E+01	59.10	E032	1 2 1 2 2	
6.405E-01	9.934E+01	61.70	E032	1 2 1 2 2	
7.163E-01	1.111E+02	64.20	E032	1 2 1 2 2	
8.409E-01	1.304E+02	65.00	E032	1 2 1 2 2	
1.074E+00	1.667E+02	93.80	E032	1 2 1 2 2	

681. $C_6H_5NO_4$

4-Nitroresorcinol
4-Nitro-1,3-benzenediol

RN: 3163-07-3 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.354E-02	6.754E+00	18.30	E032	1 2 1 2 2	
5.244E-02	8.133E+00	24.70	E032	1 2 1 2 2	
6.510E-02	1.010E+01	30.80	E032	1 2 1 2 2	
7.959E-02	1.235E+01	36.90	E032	1 2 1 2 2	
1.034E-01	1.604E+01	43.50	E032	1 2 1 2 2	
1.462E-01	2.267E+01	47.50	E032	1 2 1 2 2	
1.817E-01	2.818E+01	49.10	E032	1 2 1 2 2	
2.168E-01	3.363E+01	50.70	E032	1 2 1 2 2	
2.497E-01	3.874E+01	51.20	E032	1 2 1 2 2	
2.776E-01	4.306E+01	52.30	E032	1 2 1 2 2	
3.286E-01	5.096E+01	53.90	E032	1 2 1 2 2	
4.487E-01	6.959E+01	57.80	E032	1 2 1 2 2	
5.951E-01	9.231E+01	62.70	E032	1 2 1 2 2	
8.468E-01	1.313E+02	68.40	E032	1 2 1 2 2	
1.075E+00	1.667E+02	71.90	E032	1 2 1 2 2	
1.209E+00	1.875E+02	72.90	E032	1 2 1 2 2	
1.325E+00	2.055E+02	73.30	E032	1 2 1 2 2	
1.487E+00	2.307E+02	73.40	E032	1 2 1 2 2	

682. $C_6H_5NO_4$

2-Nitroresorcinol
2-Nitro-1,3-benzenediol

RN: 601-89-8 **MP** (°C)**:** 81
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.435E-03	1.308E+00	28.40	E032	1 2 1 2 2	
1.306E-02	2.026E+00	36.70	E032	1 2 1 2 2	
2.319E-02	3.597E+00	47.60	E032	1 2 1 2 2	
3.635E-02	5.638E+00	54.90	E032	1 2 1 2 2	

(*continued*)

682. $C_6H_5NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.276E-02	9.734E+00	67.20	E032	1 2 1 2 2	
8.399E-02	1.303E+01	74.40	E032	1 2 1 2 2	
1.208E-01	1.874E+01	82.90	E032	1 2 1 2 2	
1.529E-01	2.372E+01	92.30	E032	1 2 1 2 2	

683. $C_6H_5NO_4$

3-Nitrocatechol
3-Nitro-1,2-benzenediol
RN: 6665-98-1 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.377E-02	8.340E+00	14.40	E032	1 2 1 2 2	
6.573E-02	1.019E+01	20.90	E032	1 2 1 2 2	
9.590E-02	1.488E+01	29.50	E032	1 2 1 2 2	
1.277E-01	1.980E+01	35.10	E032	1 2 1 2 2	
1.474E-01	2.286E+01	37.90	E032	1 2 1 2 2	
1.738E-01	2.695E+01	41.00	E032	1 2 1 2 2	
2.372E-01	3.679E+01	45.80	E032	1 2 1 2 2	
2.646E-01	4.104E+01	47.60	E032	1 2 1 2 2	
3.216E-01	4.988E+01	54.50	E032	1 2 1 2 2	
3.615E-01	5.607E+01	61.30	E032	1 2 1 2 2	
4.548E-01	7.055E+01	75.90	E032	1 2 1 2 2	
5.743E-01	8.909E+01	86.80	E032	1 2 1 2 2	
8.164E-01	1.266E+02	96.80	E032	1 2 1 2 2	

684. $C_6H_5NO_4$

4-Nitrocatechol
4-Nitro-1,2-benzenediol
RN: 3316-09-4 **MP** (°C)**:**
MW: 155.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E+00	1.878E+02	24.60	E032	1 2 1 2 2	
1.423E+00	2.208E+02	37.70	E032	1 2 1 2 2	
1.488E+00	2.308E+02	41.30	E032	1 2 1 2 2	
1.664E+00	2.582E+02	51.90	E032	1 2 1 2 2	
1.829E+00	2.837E+02	58.50	E032	1 2 1 2 2	
2.004E+00	3.109E+02	66.50	E032	1 2 1 2 2	
2.049E+00	3.179E+02	67.80	E032	1 2 1 2 2	
2.149E+00	3.334E+02	71.20	E032	1 2 1 2 2	

685. $C_6H_5NO_5S$

p-Nitrobenzenesulfonic acid
4-Nitrobenzenesulfonic acid
RN: 138-42-1 **MP** (°C)**:**
MW: 203.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E+00	4.760E+02	100.5	T023	1 2 2 1 2	
2.412E+00	4.901E+02	105.0	T023	1 2 2 1 2	
2.461E+00	5.000E+02	110.0	T023	1 2 2 1 2	

686. $C_6H_5NO_5S.2H_2O$

p-Nitrobenzenesulfonic acid (dihydrate)
RN: 15481-55-7 **MP** (°C)**:**
MW: 239.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E+00	3.987E+02	36.6	T023	1 2 2 1 2	
1.720E+00	4.113E+02	56.6	T023	1 2 2 1 2	
1.771E+00	4.235E+02	75.5	T023	1 2 2 1 2	
1.822E+00	4.359E+02	90.2	T023	1 2 2 1 2	
1.939E+00	4.638E+02	106.8	T023	1 2 2 1 2	
1.920E+00	4.592E+02	110.2	T023	1 2 2 1 2	

687. $C_6H_5NO_5S.4H_2O$

p-Nitrobenzenesulfonic acid (tetrahydrate)
RN: 15481-55-7 **MP** (°C)**:**
MW: 275.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E+00	2.919E+02	–8.3	T023	1 2 2 1 2	
1.146E+00	3.153E+02	–1.0	T023	1 2 2 1 2	
1.273E+00	3.504E+02	10.8	T023	1 2 2 1 2	
1.318E+00	3.627E+02	16.0	T023	1 2 2 1 2	
1.409E+00	3.877E+02	26.3	T023	1 2 2 1 2	

688. $C_6H_5N_2OS$

Methyl acetylthiodiazole
Thiodiazolique methyle acetyle
RN: **MP** (°C)**:**
MW: 153.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.528E-04	1.000E-01	37	D084	1 0 1 0 1	

689. $C_6H_5N_3$
Benzotriazole
1,2,3-Benzotriazole
Cobratec 99
1,2,3-triaza-1H-indene
Azimidobenzene
Benzene azimide
RN: 95-14-7 **MP** (°C)**:** 98.5
MW: 119.13 **BP** (°C)**:** 350

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-01	1.977E+01	ns	R427	0 0 0 0 0	

690. $C_6H_5N_3O_4$
2,6-Dinitroaniline
2,6-Dinitrobenzenamine
RN: 606-22-4 **MP** (°C)**:** 133
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	7.994E-02	25	B335	1 2 0 0 1	

691. $C_6H_5N_3O_4$
2,4-Dinitroaniline
2,4-Dinitrobenzenamine
2,4-Dinitroaminobenzene
1-Amino-2,4-dinitrobenzene
RN: 97-02-9 **MP** (°C)**:** 176
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-04	7.812E-02	25	B335	1 2 0 0 1	

692. $C_6H_5N_3O_5$
Picramic acid
2-Amino-4,6-dinitro-phenol
RN: 96-91-3 **MP** (°C)**:** 169
MW: 199.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-03	1.400E+00	22	F300	1 0 0 0 1	

693. $C_6H_5N_5$
7-Aminopteridine
7-Pteridinamine
RN: 769-66-4 **MP** (°C)**:**
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	20	A083	1 2 0 0 0	
3.974E-02	5.848E+00	100	A083	1 2 0 0 0	

694. $C_6H_5N_5$
4-Aminopteridine
4-Pteridinamine
RN: 6973-01-9 **MP** (°C)**:** 305
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	22.5	A085	1 2 0 0 0	

695. $C_6H_5N_5$
2-Aminopteridine
2-Pteridinamine
RN: 700-81-2 **MP** (°C)**:**
MW: 147.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.031E-03	7.402E-01	22.5	A085	1 2 0 0 0	

696. $C_6H_5N_5O$
4-Amino-2-hydroxypteridine
4-Amino-2-oxopteridine
4-Aminopteridin-2-one
4-Amino-2-pteridone
RN: 22005-65-8 **MP** (°C)**:** >350
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.378E-04	7.142E-02	20	A019	2 2 1 1 2	
5.104E-03	8.326E-01	100	A019	1 2 1 1 2	

697. $C_6H_5N_5O$
2-Amino-4-hydroxypteridine
2-Amino-4(1H)-pteridinone
2-Amino-4(3H)-pteridinone
2-Amino-4-pteridone
2-Amino-4-oxopteridine
2-Aminopteridin-4-one
RN: 2236-60-4 **MP** (°C)**:**
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.075E-04	1.754E-02	22.5	A085	1 2 0 0 0	

698. $C_6H_5N_5O$
7-Amino-6-hydroxypteridine
7-Amino-6-oxopteridine
7-Aminopteridin-6-one
7-Amino-6-pteridone
RN: 1008-85-1 **MP** (°C)**:**
MW: 163.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	2.000E-01	100	A082	1 2 0 0 0	

699. $C_6H_5N_5O_2$
Xanthopterin
2-Amino-4:6-dihydroxypteridine
RN: 119-44-8 **MP** (°C)**:**
MW: 179.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.396E-04	2.500E-02	22.5	A085	1 2 0 0 0	

700. $C_6H_5N_5O_3$
Leucopterin
2-Amino-4:6:7-trihydroxypteridine
RN: 492-11-5 **MP** (°C)**:**
MW: 195.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.833E-06	1.333E-03	22.5	A085	1 2 0 0 0	

701. $C_6H_5N_5O_4S$
3′-Nitrosoniridazole
2-Imidazolidinone, 1-nitroso-3-(5-nitro-2-thiazolyl)-
RN: 34968-90-6 **MP** (°C)**:** 202-203
MW: 243.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.084E-04	7.500E-02	25	G051	1 0 1 1 0	

702. C_6H_6
Benzene
Benzol
Phenyl hydride
Cyclohexatriene
Benzolene
Phene
RN: 71-43-2 **MP** (°C)**:** 5
MW: 78.11 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E-02	1.836E+00	.20	M151	2 1 2 2 2	
2.347E-02	1.833E+00	.24	M183	1 2 1 1 2	
1.959E-02	1.530E+00	0	F300	1 0 0 0 2	
2.148E-02	1.678E+00	0	P003	2 2 2 2 2	
2.356E-02	1.840E+00	.80	A004	1 2 2 1 2	
2.351E-02	1.837E+00	4.50	B086	2 1 2 2 2	
1.881E-02	1.469E+00	4.62	U013	1 0 0 0 0	EFG
2.646E-02	2.067E+00	4.8	L007	2 1 1 2 2	
1.178E-02	9.200E-01	5	S119	0 0 0 0 1	
2.646E-02	2.067E+00	5.0	L007	2 1 1 1 2	
1.838E-02	1.436E+00	5.39	U010	1 0 0 1 1	EFG
2.310E-02	1.804E+00	6.20	M151	2 1 2 2 2	
2.306E-02	1.802E+00	6.24	M183	1 2 1 1 2	
2.364E-02	1.847E+00	6.30	B086	2 1 2 2 2	
2.313E-02	1.807E+00	7.10	B086	2 1 2 2 2	
2.313E-02	1.807E+00	9	B086	2 1 2 2 2	
2.292E-02	1.790E+00	9.40	A004	1 2 2 1 2	
2.080E-02	1.625E+00	10	B149	2 1 1 2 2	
2.110E-02	1.648E+00	10	J302	2 1 2 2 2	
2.240E-02	1.750E+00	10	M130	1 0 0 0 2	
2.300E-02	1.797E+00	11.00	M151	2 1 2 2 2	
2.300E-02	1.796E+00	11.04	M183	1 2 1 1 2	
2.262E-02	1.767E+00	11.80	B086	2 1 2 2 2	
2.262E-02	1.767E+00	12.10	B086	2 1 2 2 2	
2.270E-02	1.773E+00	14.00	M151	2 1 2 2 2	
2.263E-02	1.767E+00	14.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	14.20	U013	1 0 0 0 0	EFG
2.655E-02	2.074E+00	14.8	L007	2 1 1 2 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.655E-02	2.074E+00	14.9	L007	2 1 1 1 2	
2.290E-02	1.789E+00	15	I333	1 2 1 1 2	
2.150E-02	1.679E+00	15	S006	1 0 0 0 2	
1.971E-02	1.540E+00	15	S203	1 1 2 1 2	
1.797E-02	1.403E+00	15.02	U010	1 0 0 1 1	EFG
2.287E-02	1.787E+00	15.10	B086	2 1 2 2 2	
2.112E-02	1.650E+00	16	D047	1 0 0 1 2	
2.266E-02	1.770E+00	16.80	A004	1 2 2 1 2	
2.260E-02	1.765E+00	16.90	M151	2 1 2 2 2	
2.253E-02	1.760E+00	16.94	M183	1 2 1 1 2	
2.191E-02	1.711E+00	17	F002	2 2 2 2 2	
2.287E-02	1.787E+00	17.90	B086	2 1 2 2 2	
2.260E-02	1.765E+00	18.60	M151	2 1 2 2 2	
2.259E-02	1.764E+00	18.64	M183	1 2 1 1 2	
2.664E-02	2.081E+00	19.8	L007	2 1 1 2 2	
2.664E-02	2.081E+00	19.9	L007	2 1 1 1 2	
2.220E-02	1.734E+00	20	B149	2 1 1 2 2	
2.180E-02	1.703E+00	20	C006	1 2 1 1 2	
1.023E-02	7.994E-01	20	C121	0 0 0 0 0	unit assumed, *sic*
2.428E-02	1.896E+00	20	D052	1 1 0 0 1	
1.600E-02	1.250E+00	20	E009	1 0 0 0 1	
1.680E-02	1.312E+00	20	E025	1 0 2 2 2	
2.189E-02	1.710E+00	20	F071	1 1 2 1 2	
2.317E-02	1.810E+00	20	F300	1 0 0 0 2	
1.023E-02	7.994E-01	20	I310	0 0 0 0 0	
2.310E-02	1.804E+00	20	I333	1 2 1 1 2	
2.042E-02	1.595E+00	20	K337	1 0 0 0 2	
2.280E-02	1.781E+00	20	M312	1 0 0 0 1	
1.366E-02	1.067E+00	20	M337	2 1 2 2 2	
2.650E-02	2.070E+00	20	P073	1 0 0 1 2	
1.751E-02	1.368E+00	20.0	H043	2 2 2 2 2	
2.249E-02	1.757E+00	20.10	B086	2 1 2 2 2	
2.224E-02	1.737E+00	21	C024	2 1 1 2 2	
2.202E-02	1.720E+00	22	F002	2 2 2 2 2	
2.320E-02	1.812E+00	22.5	I333	1 2 1 1 2	
2.304E-02	1.800E+00	24	A004	1 2 2 1 2	
2.667E-02	2.084E+00	24.8	L007	2 1 1 2 2	
2.227E-02	1.740E+00	25	A001	1 2 2 2 2	
1.917E-02	1.498E+00	25	A037	2 2 2 2 2	
2.292E-02	1.790E+00	25	B003	2 2 2 2 2	
2.045E-02	1.597E+00	25	B019	1 0 1 2 0	
2.279E-02	1.780E+00	25	B060	2 0 1 1 1	
2.292E-02	1.790E+00	25	B090	2 2 2 1 2	
2.292E-02	1.790E+00	25	B151	1 2 2 1 2	
2.330E-02	1.820E+00	25	B153	2 1 1 1 2	
2.240E-02	1.750E+00	25	B173	2 0 2 2 2	
2.300E-02	1.797E+00	25	G323	2 2 2 2 2	
2.300E-02	1.797E+00	25	H332	2 2 2 2 1	
2.330E-02	1.820E+00	25	I333	1 2 1 1 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-02	1.804E+00	25	J302	2 1 2 2 2	
2.390E-02	1.867E+00	25	K001	2 2 2 2 2	
8.961E-03	7.000E-01	25	K072	1 0 1 1 1	
1.300E-02	1.015E+00	25	K123	1 0 2 2 1	
2.170E-02	1.695E+00	25	K316	2 2 2 2 2	
2.259E-02	1.765E+00	25	L002	2 2 2 2 2	
2.313E-02	1.807E+00	25	L319	1 0 2 1 1	
2.166E-02	1.692E+00	25	L322	1 1 2 2 1	
1.770E+00	1.383E+02	25	M021	2 2 2 1 2	*sic*
2.279E-02	1.780E+00	25	M131	1 0 0 0 2	
2.278E-02	1.780E+00	25	M132	2 2 2 1 2	
2.310E-02	1.804E+00	25	M151	2 1 2 2 2	average of 2
2.293E-02	1.791E+00	25	M151	2 1 1 2 2	
2.290E-02	1.789E+00	25	M342	1 0 1 1 2	
1.917E-02	1.498E+00	25	O015	0 0 0 0 0	
2.247E-02	1.755E+00	25	P003	2 2 2 2 2	
2.227E-02	1.740E+00	25	P051	2 1 1 2 2	
2.607E-02	2.036E+00	25	S010	2 1 2 1 2	
2.377E-02	1.857E+00	25	S012	2 0 2 2 2	
2.061E-02	1.610E+00	25	S203	1 1 2 1 2	
2.070E-02	1.617E+00	25	S359	2 1 2 2 2	
2.778E-02	2.170E+00	25	W057	2 0 2 2 2	
2.290E-02	1.789E+00	25	W300	2 2 2 2 2	
2.300E-02	1.797E+00	25.0	H043	2 2 2 2 2	
2.667E-02	2.084E+00	25.0	L007	2 1 1 1 2	
2.227E-02	1.740E+00	25.00	P007	2 1 2 2 2	
2.290E-02	1.789E+00	25.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	25.35	U010	1 0 0 1 1	EFG
1.881E-02	1.469E+00	25.35	U013	1 0 0 0 0	EFG
2.325E-02	1.816E+00	25.84	M183	1 2 1 1 2	
2.213E-02	1.729E+00	26	F002	2 2 2 2 2	
2.229E-02	1.742E+00	29	F002	2 2 2 2 2	
2.351E-02	1.837E+00	29.99	C349	0 0 0 0 0	
2.368E-02	1.850E+00	30	F300	1 0 0 0 2	
2.364E-02	1.847E+00	30	G029	1 0 2 2 2	
2.350E-02	1.836E+00	30	I333	1 2 1 1 2	
2.343E-02	1.830E+00	31	A004	1 2 2 1 2	
2.285E-02	1.785E+00	32	F002	2 2 2 2 2	
1.970E-02	1.539E+00	34.53	U013	1 0 0 0 0	EFG
2.685E-02	2.098E+00	34.8	L007	2 1 1 2 2	
2.329E-02	1.819E+00	35	F002	2 2 2 2 2	
2.253E-02	1.760E+00	35	S203	1 1 2 1 2	
2.685E-02	2.098E+00	35.1	L007	2 1 1 1 2	
1.925E-02	1.504E+00	35.48	U010	1 0 0 1 1	EFG
2.458E-02	1.920E+00	38	A004	1 2 2 1 2	
2.573E-02	2.010E+00	39.99	C349	0 0 0 0 0	
2.592E-02	2.025E+00	40	B151	1 2 1 1 2	
2.434E-02	1.902E+00	41	F002	2 2 2 2 2	
2.440E-02	1.906E+00	42	F002	2 2 2 2 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.467E-02	1.927E+00	44	F002	2 2 2 2 2	
2.016E-02	1.574E+00	44.30	U010	1 0 0 1 1	EFG
2.062E-02	1.611E+00	44.30	U013	1 0 0 0 0	EFG
2.599E-02	2.030E+00	44.70	A004	1 2 2 1 2	
2.368E-02	1.850E+00	45	S203	1 1 2 1 2	
2.938E-02	2.295E+00	45.7	L007	2 1 1 1 2	
2.938E-02	2.295E+00	45.8	L007	2 1 1 2 2	
2.534E-02	1.979E+00	46	F002	2 2 2 2 2	
2.827E-02	2.208E+00	49.99	C349	0 0 0 0 0	
2.810E-02	2.195E+00	50	G323	2 2 2 2 1	
2.650E-02	2.070E+00	51	F002	2 2 2 2 2	
2.740E-02	2.140E+00	51.50	A004	1 2 2 1 2	
2.159E-02	1.687E+00	53.64	U010	1 0 0 1 1	EFG
2.210E-02	1.726E+00	54.71	U013	1 0 0 0 0	EFG
5.095E-02	3.980E+00	55.3	P051	2 1 1 2 2	
5.095E-02	3.980E+00	55.30	P007	2 1 2 2 2	
2.788E-02	2.178E+00	56	F002	2 2 2 2 2	
3.162E-02	2.470E+00	57	B124	2 2 2 1 2	
3.776E-02	2.950E+00	57.70	B124	1 2 2 1 2	
2.996E-02	2.340E+00	58.80	A004	1 2 2 1 2	
3.131E-02	2.446E+00	59.99	C349	0 0 0 0 0	
2.938E-02	2.295E+00	60	B126	1 0 1 1 1	
3.101E-02	2.422E+00	60	B151	1 2 1 1 2	
2.943E-02	2.299E+00	61	F002	2 2 2 2 2	
3.004E-02	2.347E+00	63	F002	2 2 2 2 2	
3.290E-02	2.570E+00	65.40	A004	1 2 2 1 2	
2.479E-02	1.936E+00	65.82	U013	1 0 0 0 0	EFG
3.597E-02	2.810E+00	69.20	B124	1 2 2 1 2	
3.587E-02	2.802E+00	69.30	B124	1 0 2 2 2	
3.463E-02	2.705E+00	69.99	C349	0 0 0 0 0	
8.280E-02	6.468E+00	74.7	P051	2 1 1 2 2	
8.280E-02	6.468E+00	74.70	P007	2 1 2 2 2	
3.872E-02	3.024E+00	79.99	C349	0 0 0 0 0	
4.429E-02	3.460E+00	89.99	C349	0 0 0 0 0	
2.560E-02	2.000E+00	100	J023	1 1 2 2 0	
5.256E-02	4.106E+00	99.99	C349	0 0 0 0 0	
7.681E-02	6.000E+00	150	J023	1 1 2 2 0	
2.688E-01	2.100E+01	200	J023	1 1 2 2 1	
9.345E-01	7.300E+01	250	J023	1 1 2 2 1	
1.357E+00	1.060E+02	285	J023	1 1 2 2 2	
1.869E+00	1.460E+02	300	J023	1 1 2 2 2	
2.200E-02	1.719E+00	ns	B059	0 0 1 1 2	
4.000E-03	3.125E-01	ns	D348	0 0 0 0 0	
2.279E-02	1.780E+00	ns	H123	0 0 0 0 0	
3.020E-01	2.359E+01	ns	H307	0 0 0 0 0	
4.500E-02	3.515E+00	ns	H333	0 1 0 1 0	EFG
2.330E-02	1.820E+00	ns	I332	0 0 0 0 2	
2.292E-02	1.790E+00	ns	K304	0 0 0 0 2	
1.933E-02	1.510E+00	ns	M010	0 0 0 0 2	

(*continued*)

702. C_6H_6 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-02	1.769E+00	ns	M175	0 0 2 1 2	
2.279E-02	1.780E+00	ns	M344	0 0 0 0 2	

703. $C_6H_6BrNO_2S$

4-Bromobenzenesulfonamide
(4-Bromophenyl)sulfonamide
p-Bromobenzenesulfonamide
4-Aminosulfonyl-1-bromobenzene
RN: 701-34-8 **MP** (°C)**:**
MW: 236.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	9.916E-01	15	K024	1 2 1 1 2	

704. $C_6H_6BrNO_3S$

p-Bromoaniline-*o*-sulfonic acid
2-Amino-5-bromophenylsulfonic acid
RN: 1576-59-6 **MP** (°C)**:**
MW: 252.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.107E-02	2.790E+00	8.35	P038	1 0 1 0 2	anhydrate
1.424E-02	3.590E+00	16.75	P038	1 0 1 0 2	anhydrate
1.769E-02	4.460E+00	25.0	P038	1 0 1 0 2	anhydrate
2.578E-02	6.500E+00	40.0	P038	1 0 1 0 2	anhydrate
3.828E-02	9.650E+00	55.0	P038	1 0 1 0 2	anhydrate
5.454E-02	1.375E+01	70.0	P038	1 0 1 0 2	anhydrate
8.013E-02	2.020E+01	85.0	P038	1 0 1 0 2	anhydrate
8.846E-03	2.230E+00	.0	P038	1 0 1 0 2	anhydrate

705. $C_6H_6BrNO_3S$

p-Bromoaniline-*m*-sulfonic acid
5-Amino-2-bromobenzenesulfonic acid
RN: 150454-14-1 **MP** (°C)**:**
MW: 252.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E-02	8.850E+00	9.8	P038	1 2 2 2 2	anhydrous rhombic
2.559E-02	6.450E+00	12.55	P038	1 2 2 2 2	anhydrous monoclinic
4.284E-02	1.080E+01	20.0	P038	1 2 2 2 2	anhydrous rhombic
3.419E-02	8.620E+00	25.0	P038	1 2 2 2 2	anhydrous monoclinic
4.740E-02	1.195E+01	25.0	P038	1 2 2 2 2	anhydrous rhombic
5.177E-02	1.305E+01	29.6	P038	1 2 2 2 2	anhydrous rhombic
5.732E-02	1.445E+01	34.7	P038	1 2 2 2 2	anhydrous rhombic
4.820E-02	1.215E+01	40.0	P038	1 2 2 2 2	anhydrous monoclinic

(*continued*)

705. $C_6H_6BrNO_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.387E-02	1.610E+01	40.1	P038	1 2 2 2 2	anhydrous rhombic
6.922E-02	1.745E+01	44.5	P038	1 2 2 2 2	anhydrous rhombic
7.577E-02	1.910E+01	49.7	P038	1 2 2 2 2	anhydrous rhombic
8.330E-02	2.100E+01	54.8	P038	1 2 2 2 2	anhydrous rhombic
7.101E-02	1.790E+01	56.3	P038	1 2 2 2 2	anhydrous monoclinic
9.600E-02	2.420E+01	62.3	P038	1 2 2 2 2	anhydrous rhombic
9.679E-02	2.440E+01	70.0	P038	1 2 2 2 2	anhydrous monoclinic
1.115E-01	2.810E+01	70.4	P038	1 2 2 2 2	anhydrous rhombic
1.329E-01	3.350E+01	85.0	P038	1 2 2 2 2	anhydrous monoclinic
1.452E-01	3.660E+01	85.0	P038	1 2 2 2 2	anhydrous rhombic
2.880E-02	7.260E+00	.0	P038	1 2 2 2 2	anhydrous rhombic
1.884E-02	4.750E+00	.0	P038	1 2 2 2 2	anhydrous monoclinic

706. $C_6H_6BrNO_3S.H_2O$

p-Bromoaniline-*o*-sulfonic acid (monohydrate)
2-Amino-5-bromophenylsulfonic acid (monohydrate)
RN: 1576-59-6 **MP** (°C)**:**
MW: 270.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.520E+00	8.35	P038	1 0 1 0 2	monohydrate
1.751E-02	4.730E+00	16.8	P038	1 0 1 0 2	monohydrate
2.244E-02	6.060E+00	25.0	P038	1 0 1 0 2	monohydrate
9.589E-03	2.590E+00	.0	P038	1 0 1 0 2	monohydrate

707. C_6H_6ClN

p-Chloroaniline
4-Chloroaniline
RN: 106-47-8 **MP** (°C)**:** 72.5
MW: 127.57 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.157E-02	2.752E+00	20	H118	1 1 1 1 2	
2.157E-02	2.752E+00	20	H301	0 0 0 0 0	
3.057E-02	3.900E+00	22.5	G301	0 0 0 0 0	

708. C_6H_6ClN

o-Chloroaniline
2-Chloroaniline
RN: 95-51-2 **MP** (°C)**:** –1
MW: 127.57 **BP** (°C)**:** 208.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-02	3.765E+00	20	C113	1 0 2 1 2	

709. C_6H_6ClN
m-Chloroaniline
3-Chloroaniline
RN: 108-42-9 **MP** (°C)**:** –10
MW: 127.57 **BP** (°C)**:** 230.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-02	5.442E+00	20	C113	1 0 2 1 2	

710. $C_6H_6ClNO_2S$
m-Chlorobenzenesulfonamide
MON 5783
RN: 17260-71-8 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	6.707E-01	15	K024	1 2 1 1 2	

711. $C_6H_6ClNO_2S$
o-Chlorobenzenesulfonamide
2-Chlorobenzenesulfonamide
RN: 6961-82-6 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.983E-01	15	K024	1 2 1 1 2	

712. $C_6H_6ClNO_2S$
4-Chlorobenzenesulfonamide
p-Chlorobenzenesulfonamide
RN: 98-64-6 **MP** (°C)**:**
MW: 191.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.322E+00	15	K024	1 2 1 1 2	

713. $C_6H_6ClNO_3S$
p-Chloroaniline-*m*-sulfonic acid
1-Amino-4-chlorobenzene-3-sulfonic acid
4-Chloro-3-sulfoaniline
3-Amino-6-chlorobenzenesulfonic acid
RN: 88-43-7 **MP** (°C)**:**
MW: 207.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.447E-02	1.131E+01	0	P038	1 0 1 1 2	anhydrate

714. $C_6H_6ClNO_3S.H_2O$

p-Chloroaniline-*o*-sulfonic acid (monohydrate)
1-Amino-4-chloro-2-benzenesulfonic acid (monohydrate)
RN: 133-74-4 **MP** (°C)**:**
MW: 225.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.387E-02	3.130E+00	0	P038	1 2 2 1 2	monohydrate

715. $C_6H_6ClNO_3S.H_2O$

p-Chloroaniline-*m*-sulfonic acid (monohydrate)
1-Amino-4-chlorobenzene-3-sulfonic acid (monohydrate)
RN: 88-43-7 **MP** (°C)**:**
MW: 225.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.141E-02	1.160E+01	0	P038	1 0 1 1 2	metastable monohydrate

716. $C_6H_6Cl_6$

β-1,2,3,4,5,6-Hexachlorocyclohexane
β-Benzene hexachloride
β-BHC
β-Hexachlorocyclohexane
RN: 319-85-7 **MP** (°C)**:** 312
MW: 290.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-05	5.000E-03	20	C099	1 2 0 0 0	
8.252E-07	2.400E-04	25	W025	1 0 2 2 2	
5.501E-07	1.600E-04	28	K120	1 2 2 2 1	average of 2
1.719E-06	5.000E-04	ns	M061	0 0 0 0 0	

717. $C_6H_6Cl_6$

δ-1,2,3,4,5,6-Hexachlorocyclohexane
δ-Benzene hexachloride
RN: 608-73-1 **MP** (°C)**:**
MW: 290.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
1.080E-04	3.140E-02	25	W025	1 0 2 2 2	
4.009E-05	1.166E-02	28	K120	1 2 2 2 2	average of 4

718. $C_6H_6Cl_6$

Lindane
γ-BHC
Benzene hexachloride

RN: 58-89-9 **MP** (°C)**:** 112.5
MW: 290.83 **BP** (°C)**:** 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.393E-06	2.150E-03	15	B083	2 2 1 2 2	
7.393E-06	2.150E-03	15	B162	1 0 0 0 2	
2.816E-05	8.190E-03	19	I018	1 0 0 0 2	
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
2.709E-05	7.880E-03	22	K137	1 1 2 1 0	
2.706E-05	7.870E-03	24	C313	0 0 0 0 0	
5.845E-05	1.700E-02	24	H116	2 1 0 0 2	
2.338E-05	6.800E-03	25	B083	2 2 1 2 2	
2.338E-05	6.800E-03	25	B162	1 0 0 0 2	
2.586E-05	7.520E-03	25	M060	2 2 1 2 2	
2.510E-05	7.300E-03	25	M130	1 0 0 0 1	
2.682E-05	7.800E-03	25	W025	1 0 2 2 2	
4.126E-05	1.200E-02	27	B161	2 1 2 2 0	EFG
2.235E-05	6.500E-03	28	K120	1 2 2 2 2	average of 4
3.920E-05	1.140E-02	35	B083	2 2 1 2 2	particle size 5 µm
7.221E-05	2.100E-02	35	B161	2 1 2 2 0	EFG
3.920E-05	1.140E-02	35	B162	1 0 0 0 2	
5.226E-05	1.520E-02	45	B083	2 2 1 2 2	particle size 5 µm
9.284E-05	2.700E-02	45	B161	2 1 2 2 0	EFG
1.135E-04	3.300E-02	50	B161	2 1 2 2 0	EFG
1.547E-04	4.500E-02	60	B161	2 1 2 2 0	EFG
2.400E-05	6.980E-03	ns	C318	0 0 0 0 0	
~3.44E-05	~1.00E-02	ns	I308	0 0 0 0 0	
5.158E-07	1.500E-04	ns	K138	0 0 0 0 2	*sic*
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	
2.407E-05	7.000E-03	ns	M110	0 0 0 0 0	EFG
2.510E-05	7.300E-03	ns	V414	0 0 0 0 0	
3.438E-05	1.000E-02	rt	M161	0 0 0 0 1	

719. $C_6H_6Cl_6$

α-1,2,3,4,5,6-Hexachlorocyclohexane
α-Benzene hexachloride
α-HCH
α-BHC
α-Hexachlorocyclohexane

RN: 319-84-6 **MP** (°C)**:** 158
MW: 290.83 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
6.877E-06	2.000E-03	25	W025	1 0 2 2 2	
5.570E-06	1.620E-03	28	K120	1 2 2 2 2	average of 4
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	

720. $C_6H_6FN_3O_3$
1-Methylcarbamoyl-5-fluorouracil
5-Fluoro-3,4-dihydro-*N*-methyl-2,4-dioxo-pyrimidinecarboxamide
1-Methylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
RN: 56563-18-9 **MP** (°C)**:** 225–228
MW: 187.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	6.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.313E-03	6.200E-01	22	B388	0 0 0 0 0	

721. $C_6H_6INO_3S$
2-Iodoaniline-4-sulphonic acid
Benzenesulfonic acid, 4-amino-2-iodo-
RN: 67877-88-7 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.781E-02	2.028E+01	25	B107	1 2 1 1 2	

722. $C_6H_6INO_3S$
3-Iodoaniline-4-sulphonic acid
Benzenesulfonic acid, 4-amino-3-iodo-
RN: 25210-30-4 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-03	1.936E+00	25	B107	1 2 1 1 2	

723. $C_6H_6INO_3S$
4-Iodoaniline-2-sulphonic acid
Benzenesulfonic acid, 2-amino-4-iodo-
RN: 171664-62-3 **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.697E-02	5.074E+00	25	B107	1 2 1 1 1	

724. $C_6H_6INO_3S$
4-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-4-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.486E-02	1.342E+01	25	B107	1 2 1 1 2	

725. $C_6H_6INO_3S$
5-Iodoaniline-2-sulphonic acid
Benzenesulfonic acid, 2-amino-5-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.671E-03	2.593E+00	25	B107	1 2 1 1 1	

726. $C_6H_6INO_3S$
6-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-6-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.597E-02	4.777E+00	25	B107	1 2 1 1 1	

727. $C_6H_6INO_3S$
5-Iodoaniline-3-sulphonic acid
Benzenesulfonic acid, 3-amino-5-iodo-
RN: **MP** (°C)**:**
MW: 299.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-02	1.293E+01	25	B107	1 2 1 1 2	

728. $C_6H_6N_2O$
Nicotiamide
Niacinamide
Nicotinamide
RN: 98-92-0 **MP** (°C)**:** 131
MW: 122.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.094E+00	5.000E+02	20	D041	1 0 0 0 2	
8.188E+00	1.000E+03	20	M054	1 0 0 0 2	
2.900E-03	3.542E-01	25	A350	0 0 0 0 0	
8.188E+00	1.000E+03	25	D315	0 0 0 0 0	
8.188E-01	1.000E+02	ns	K444	0 0 0 0 0	

729. $C_6H_6N_2O_2$
3-Nitroaniline
1-Amino-3-nitrobenzene
3-Nitrobenzenamine
m-Nitroaminobenzene
m-Nitroaniline
3-Nitro-anilin
RN: 99-09-2 **MP** (°C)**:** 114
MW: 138.13 **BP** (°C)**:** 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-03	1.203E+00	20	B179	0 0 0 0 0	
5.370E-03	7.418E-01	25	B335	1 2 0 0 1	
6.516E-03	9.000E-01	25	F300	1 0 0 0 2	
3.020E-03	4.171E-01	25	L016	1 0 0 0 2	unit assumed
6.582E-03	9.092E-01	25.0	C026	0 0 0 0 0	
1.290E-02	1.782E+00	40.1	C026	0 0 0 0 0	

730. $C_6H_6N_2O_2$
Urocanic acid
Urocaninsaeure
RN: 104-98-3 **MP** (°C)**:** 225
MW: 138.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E-02	1.500E+00	17.40	F300	1 0 0 0 1	
4.318E-02	5.964E+00	37	D041	1 0 0 0 0	
5.575E-02	7.700E+00	50	F300	1 0 0 0 1	
4.098E-01	5.660E+01	100	D041	1 0 0 0 0	

731. $C_6H_6N_2O_2$
p-Nitroaniline
4-Amino-nitrobenzene
Benzenamine
4-Nitroaniline
p-Aminonitrobenzene
4-Nitrobenzenamine
RN: 100-01-6 **MP** (°C)**:** 146
MW: 138.13 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.754E-03	7.948E-01	20	B179	0 0 0 0 0	
2.823E-03	3.900E-01	20	H300	1 2 2 2 1	*sic*
2.815E-03	3.888E-01	20	T301	1 2 2 2 2	
3.020E-03	4.171E-01	25	B335	1 2 0 0 1	
4.344E-03	6.000E-01	25	F300	1 0 0 0 2	*sic*
5.370E-03	7.418E-01	25	L016	1 0 0 0 2	unit assumed
4.110E-03	5.677E-01	25.0	C026	0 0 0 0 0	
5.267E-03	7.275E-01	30	G029	1 0 2 2 2	
8.367E-03	1.156E+00	40.1	C026	0 0 0 0 0	

732. $C_6H_6N_2O_2$
2-Nitroaniline
o-Nitroaniline
1-Amino-2-nitrobenzene
2-Nitro-aniline
RN: 88-74-4 **MP** (°C)**:** 71.5
MW: 138.13 **BP** (°C)**:** 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.467E-03	8.932E-01	20	T301	1 2 2 2 2	
8.764E-03	1.211E+00	25.0	C026	0 0 0 0 0	
1.750E-02	2.417E+00	40.1	C026	0 0 0 0 0	
6.134E-03	8.473E-01	50	T301	1 2 2 2 2	average of 4
6.799E-03	9.391E-01	80	T301	1 2 2 2 2	average of 4

733. $C_6H_6N_2O_3$
5,5-Ethylenebarbituric acid
Spirocyclopropane-1′,5-barbituric acid
5,7-Diazaspiro[2.5]octane-4,6,8-trione
Cyclopropane-spirobarbiturate
RN: 6947-77-9 **MP** (°C)**:**
MW: 154.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.004E+00	25	P350	0 0 0 0 0	intrinsic

734. $C_6H_6N_2O_4$
1-Methylorotic acid
4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-
RN: 705-36-2 **MP** (°C)**:**
MW: 170.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.042E+01	20	N019	0 0 0 0 0	

735. $C_6H_6N_2O_4S$
m-Nitrobenzenesulfonamide
3-Nitrobenzenesulfonamide
RN: 121-52-8 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	4.448E-01	15	K024	1 2 1 1 2	

736. $C_6H_6N_2O_4S$
4-Nitrobenzenesulfonamide
p-Nitrobenzenesulfonamide
RN: 6325-93-5 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.066E-01	15	K024	1 2 1 1 2	

737. $C_6H_6N_2O_4S$
2-Nitrobenzenesulfonamide
o-Nitrobenzenesulfonamide
RN: 5455-59-4 **MP** (°C)**:**
MW: 202.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	3.235E-01	15	K024	1 2 1 1 2	

738. $C_6H_6N_4$
8-Methylpurine
1H-Purine, 8-methyl-
RN: 934-33-8 **MP** (°C)**:**
MW: 134.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.924E-01	5.263E+01	20	A022	1 0 0 0 0	

739. $C_6H_6N_4O$
8-Hydroxymethylpurine
Purine-8-methanol
RN: 6642-26-8 **MP** (°C)**:**
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.014E-02	4.525E+00	20	A022	1 2 0 0 0	
4.440E-01	6.667E+01	100	A082	1 2 0 0 0	

740. $C_6H_6N_4O_3$
9-Methyluric acid
1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-9-methyl-
*N*9-Methyluric acid
RN: 55441-71-9 **MP** (°C)**:**
MW: 182.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-03	5.461E-01	ns	B115	0 0 1 1 0	

741. $C_6H_6N_4O_3$
1-Methyluric acid
α-Methyluric acid
RN: 708-79-2 **MP** (°C)**:** 400
MW: 182.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	2.101E+00	ns	B115	0 0 1 1 0	ζ form
8.701E-03	1.585E+00	ns	B115	0 0 1 1 0	γ form
2.731E-02	4.975E+00	ns	B115	0 0 1 1 0	
2.754E-02	5.017E+00	ns	R427	0 0 0 0 0	

742. $C_6H_6N_4O_3S$
Niridazole
Nirodazole
RN: 61-57-4 **MP** (°C)**:** 261
MW: 214.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.068E-04	1.300E-01	25	A081	1 0 1 1 0	EFG
1.634E-04	3.500E-02	25	G051	1 0 1 1 0	pH 2

743. $C_6H_6N_4O_4$
5-Nitro-2-furaldehyde semicarbazone
Nitrofurazone
RN: 59-87-0 **MP** (°C)**:** 236
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.225E-04	1.630E-01	ns	B404	0 2 1 1 0	
1.201E-03	2.380E-01	ns	I310	0 0 0 0 0	
8.128E-04	1.611E-01	ns	R427	0 0 0 0 0	

744. $C_6H_6N_6$
2,4-Diaminopteridine
2:4-Diaminopteridine
RN: 1127-93-1 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.055E-03	3.332E-01	20	A019	2 2 1 1 2	
4.708E-02	7.634E+00	100	A019	1 2 1 1 1	

745. $C_6H_6N_6$
4,6-Diaminopteridine
4:6-Diaminopteridine
RN: 19167-60-3 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.569E-04	4.166E-02	20	A020	1 2 0 1 1	
6.554E-03	1.063E+00	100	A020	1 2 0 0 0	

746. $C_6H_6N_6$
4,7-Diaminopteridine
4:7-Diaminopteridine
RN: 771-41-5 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
1.233E-03	2.000E-01	20	A020	1 2 0 0 1	
2.049E-02	3.322E+00	100	A020	1 2 0 0 0	

747. $C_6H_6N_6$
4-Hydrazinopteridine
4(1H)-Pteridinone, hydrazone
RN: 77632-11-2 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
1.367E-02	2.217E+00	20	A083	1 2 0 0 0	
8.686E-02	1.408E+01	100	A083	1 2 0 0 0	

748. C_6H_6O
Phenol
Carbolic acid
Hydroxybenzene
RN: 108-95-2 **MP** (°C)**:** 40.85
MW: 94.11 **BP** (°C)**:** 182

Solubility (Moles/L)	**Solubility (Grams/L)**	**Temp (°C)**	**Ref (#)**	**Evaluation (T P E A A)**	**Comments**
7.164E-01	6.743E+01	0	A056	1 0 1 1 2	
7.136E-01	6.716E+01	0	B031	1 2 2 2 1	
7.164E-01	6.743E+01	0	L059	1 0 1 1 2	
6.858E-01	6.455E+01	8.60	C058	2 0 2 1 1	
7.321E-01	6.890E+01	10	A056	1 0 1 1 2	
7.321E-01	6.890E+01	10	L059	1 0 1 1 2	
8.080E-01	7.604E+01	15.1	A400	2 1 2 2 2	

(*continued*)

748. C_6H_6O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-01	6.279E+01	16	D041	1 0 0 0 1	
7.779E-01	7.322E+01	20	B031	1 2 2 2 1	
8.710E-01	8.197E+01	20	B179	0 0 0 0 0	
4.866E+00	4.580E+02	20	C052	1 2 1 1 2	*sic*
8.235E-01	7.750E+01	20	F300	1 0 0 0 2	
8.198E-01	7.715E+01	20	H003	1 2 2 1 2	
1.600E+00	1.506E+02	20	H306	1 0 1 2 1	
8.500E-01	8.000E+01	20	K119	1 0 0 0 2	
7.130E-01	6.710E+01	20	K301	2 2 1 1 2	
6.175E-01	5.811E+01	20	R087	0 0 0 0 0	0.15M NaCl
9.490E-01	8.931E+01	22.70	M135	1 2 1 1 2	
1.000E+00	9.411E+01	25	A021	1 2 1 1 0	
8.930E-01	8.405E+01	25	A400	2 1 2 2 2	
9.882E-01	9.300E+01	25	B060	2 0 1 1 1	
9.400E-01	8.847E+01	25	B316	0 0 0 0 0	
9.000E-01	8.470E+01	25	F044	1 0 0 0 1	
8.468E-01	7.970E+01	25	H003	1 2 2 1 2	
8.245E-01	7.759E+01	25	H028	2 0 2 0 2	
1.527E-01	1.437E+01	25	K129	2 1 2 2 2	
8.854E-01	8.333E+01	25	L022	1 0 0 0 0	
9.000E-01	8.470E+01	25	L088	1 0 0 0 1	
7.413E-01	6.977E+01	25	M041	1 1 0 0 1	
9.300E-01	8.753E+01	25	P031	0 0 0 0 0	
7.688E-01	7.236E+01	25	R041	0 0 0 0 0	
9.900E-01	9.317E+01	26.90	M135	1 2 1 1 2	
8.970E-01	8.442E+01	30	H003	1 2 2 1 2	
8.297E-01	7.809E+01	30	V009	1 0 0 0 1	
1.048E+00	9.863E+01	32.20	M135	1 2 1 1 2	
9.598E-01	9.033E+01	34	B063	1 2 2 1 2	
9.892E-01	9.310E+01	35	A400	2 1 2 2 2	
9.580E-01	9.016E+01	35	H003	1 2 2 1 2	
1.107E+00	1.042E+02	36.00	M135	1 2 1 1 2	
9.130E-01	8.592E+01	40	B031	1 2 2 2 1	
1.158E+00	1.090E+02	43.70	M135	1 2 1 1 2	
1.369E+00	1.288E+02	47.70	M135	1 2 1 1 2	
1.172E+00	1.103E+02	48.00	C058	2 0 2 1 2	
1.138E+00	1.071E+02	50	M041	1 1 0 0 2	
1.476E+00	1.389E+02	50.50	M135	1 2 1 1 2	
1.183E+00	1.113E+02	51.90	B063	1 2 2 1 2	
1.592E+00	1.498E+02	53.50	M135	1 2 1 1 2	
1.725E+00	1.623E+02	55.80	M135	1 2 1 1 2	
1.388E+00	1.306E+02	55.90	B063	1 2 2 1 2	
1.375E+00	1.295E+02	57.30	H003	1 2 2 1 2	
1.856E+00	1.747E+02	57.80	M135	1 2 1 1 2	
1.590E+00	1.497E+02	60	B031	1 2 2 2 2	
2.163E+00	2.036E+02	60.90	M135	1 2 1 1 2	
1.612E+00	1.518E+02	61.70	B063	1 2 2 1 2	
1.723E+00	1.621E+02	62.74	H003	1 2 2 1 2	
1.771E+00	1.667E+02	63.20	B063	1 2 2 1 2	

(*continued*)

748. C_6H_6O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+00	1.985E+02	65.40	B063	1 2 2 1 2	
3.064E+00	2.884E+02	65.50	B063	1 2 2 1 2	
2.567E+00	2.416E+02	65.55	B063	1 2 2 1 2	
2.767E+00	2.604E+02	65.60	B063	1 2 2 1 2	
2.388E+00	2.247E+02	65.79	H003	1 2 2 1 2	average of 2
2.590E+00	2.437E+02	65.84	H003	1 2 2 1 2	
2.624E+00	2.469E+02	65.86	H003	1 2 2 1 2	
2.536E+00	2.387E+02	65.90	H003	1 2 2 1 2	
2.818E+00	2.652E+02	66.0	H068	2 0 0 0 2	
2.397E+00	2.256E+02	66.01	H003	1 2 2 1 2	
1.734E+00	1.632E+02	66.30	C058	2 0 2 1 2	
8.243E-01	7.758E+01	ns	A406	0 0 0 0 1	
8.594E-01	8.088E+01	ns	N330	2 2 2 1 2	
8.710E-01	8.197E+01	ns	R427	0 0 0 0 0	
8.043E-01	7.570E+01	rt	N051	0 0 2 1 2	average of 3

749. $C_6H_6O_2$

Hydroquinone
Hydrochinon
Hydroquinol

RN: 123-31-9 **MP** (°C)**:** 173.5
MW: 110.11 **BP** (°C)**:** 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.493E-01	3.846E+01	0	M043	1 0 0 0 1	
4.653E-01	5.123E+01	10	M043	1 0 0 0 1	
4.904E-01	5.400E+01	15	F300	1 0 0 0 1	
5.077E-01	5.590E+01	17.70	L065	1 0 0 0 2	0.01N HCl
5.087E-01	5.601E+01	17.90	L065	1 0 0 0 2	0.01N HCl
5.101E-01	5.617E+01	17.95	L065	1 0 0 0 2	0.01N HCl
5.103E-01	5.619E+01	18	L064	2 2 2 1 2	0.01N HCl
6.100E-01	6.716E+01	20	M043	1 0 0 0 1	
6.357E-01	7.000E+01	22.5	G301	0 0 0 0 0	
6.180E-01	6.805E+01	23.75	L064	2 2 2 1 2	0.01N HCl
6.450E-01	7.102E+01	25	G033	1 0 1 1 2	
7.283E-01	8.020E+01	25	K033	1 0 0 1 2	
6.660E-01	7.334E+01	25	K040	1 0 2 1 2	
7.955E-01	8.759E+01	30	M043	1 0 0 0 1	
1.045E+00	1.150E+02	40	M043	1 0 0 0 1	
2.354E+00	2.593E+02	60	M043	1 0 0 0 1	
5.694E+00	6.270E+02	75.3	W038	2 2 2 1 2	
4.251E+00	4.681E+02	80	M043	1 0 0 0 1	
7.528E+00	8.289E+02	81.9	W038	2 2 2 1 2	
6.034E+00	6.644E+02	100	M043	1 0 0 0 2	
1.961E+01	2.159E+03	114.6	W038	2 2 2 1 2	
2.180E+01	2.400E+03	120.3	W038	2 2 2 1 2	
2.728E+01	3.004E+03	131.7	W038	2 2 2 1 2	

(*continued*)

749. $C_6H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.942E+01	3.239E+03	136.0	W038	2 2 2 1 2	
3.353E+01	3.692E+03	141.8	W038	2 2 2 1 2	
3.621E+01	3.987E+03	147.2	W038	2 2 2 1 2	
6.026E-01	6.635E+01	ns	R427	0 0 0 0 0	
6.084E-01	6.699E+01	rt	D021	0 0 1 1 2	

750. $C_6H_6O_2$

Pyrocatechol
Brenzkatechin
Catechol

RN: 120-80-9 **MP** (°C)**:** 105
MW: 110.11 **BP** (°C)**:** 245.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.824E+00	3.110E+02	20	F300	1 0 0 0 2	
2.823E+00	3.108E+02	20	M043	1 0 0 0 2	
4.190E+00	4.614E+02	25	K040	1 0 2 1 2	
5.743E+00	6.324E+02	40	M043	1 0 0 0 2	
1.278E+01	1.408E+03	41.2	W038	2 2 2 1 2	
2.061E+01	2.270E+03	56.7	W038	2 2 2 1 2	
2.068E+01	2.278E+03	57.1	W038	2 2 2 1 2	
7.308E+00	8.047E+02	60	M043	1 0 0 0 2	
2.617E+01	2.882E+03	66.2	W038	2 2 2 1 2	
8.337E+00	9.180E+02	80	M043	1 0 0 0 2	
8.974E+00	9.882E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	104.5	W038	2 2 2 1 2	
2.823E+00	3.108E+02	rt	D021	0 0 1 1 2	

751. $C_6H_6O_2$

Resorcinol
Resorcin

RN: 108-46-3 **MP** (°C)**:** 110.0
MW: 110.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E+00	3.748E+02	0	M022	1 0 0 0 2	
3.617E+00	3.983E+02	0	M043	1 0 0 0 2	
2.784E+00	3.066E+02	3.70	L090	1 0 0 1 2	
4.173E+00	4.595E+02	10	M043	1 0 0 0 1	
5.413E+00	5.960E+02	12.50	F300	1 0 0 0 2	
3.186E+00	3.508E+02	14.20	L090	1 0 0 1 2	
3.359E+00	3.699E+02	19.50	L090	1 0 0 1 2	
4.576E+00	5.038E+02	20	M022	1 0 0 0 2	
5.009E+00	5.516E+02	20	M043	1 0 0 0 2	
6.515E+00	7.174E+02	25	K040	1 0 2 1 2	

(*continued*)

751. $C_6H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.330E+00	6.970E+02	30	F300	1 0 0 0 2	
5.718E+00	6.296E+02	30	M043	1 0 0 0 2	
3.679E+00	4.051E+02	32.50	L090	1 0 0 1 2	
1.464E+01	1.612E+03	33.61	W038	2 2 2 1 2	
5.641E+00	6.211E+02	40	M022	1 0 0 0 2	
6.287E+00	6.923E+02	40	M043	1 0 0 0 2	
1.843E+01	2.030E+03	44.5	W038	2 2 2 1 2	
2.042E+01	2.249E+03	49.3	W038	2 2 2 1 2	
2.100E+01	2.312E+03	50.4	W038	2 2 2 1 2	
6.465E+00	7.119E+02	60	M022	1 0 0 0 2	
7.228E+00	7.959E+02	60	M043	1 0 0 0 2	
2.701E+01	2.974E+03	64.4	W038	2 2 2 1 2	
2.997E+01	3.300E+03	70.7	W038	2 2 2 1 2	
7.106E+00	7.825E+02	80	M022	1 0 0 0 2	
7.844E+00	8.638E+02	80	M043	1 0 0 0 2	
3.516E+01	3.871E+03	80.5	W038	2 2 2 1 2	
4.008E+01	4.414E+03	88.5	W038	2 2 2 1 2	
7.592E+00	8.360E+02	100	M022	1 0 0 0 2	
8.299E+00	9.138E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	109.4	W038	2 2 2 1 2	
4.608E+00	5.074E+02	rt	D021	0 0 1 1 2	

752. $C_6H_6O_3$

Maltol
3-Hydroxy-2-methyl-4-pyrone
Hydroxymethylpyrone
Palatone

RN: 118-71-8 **MP** (°C)**:** 161.5
MW: 126.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.643E-02	1.090E+01	15	F300	1 0 0 0 2	

753. $C_6H_6O_3$

Methyl furoate
5-Methyl-brenzschleimsaeure
5-Methylfuroic acid

RN: 611-13-2 **MP** (°C)**:**
MW: 126.11 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	1.860E+01	20	F300	1 0 0 0 2	

754. $C_6H_6O_3$

Phloroglucinol
1,3,5-Benzenetriol
1,3,5-Trihydroxybenzene
1,3,5-THB

RN: 108-73-6 **MP** (°C)**:** 218.0
MW: 126.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.405E-02	1.060E+01	20	F300	1 0 0 0 2	
8.860E-02	1.117E+01	rt	D021	0 0 1 1 2	

755. $C_6H_6O_3$

Pyrogallol
1,2,3-Trihydroxybenzene
1,2,3-Benzenetriol
Brown AP
Fourrine 85

RN: 87-66-1 **MP** (°C)**:** 131
MW: 126.11 **BP** (°C)**:** 309

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	3.000E+02	13	F300	1 0 0 0 0	average
3.013E+00	3.800E+02	25	F300	1 0 0 0 1	
4.020E+00	5.070E+02	25	K040	1 0 2 1 2	

756. $C_6H_6O_3S$

Benzenesulfonic acid
Benzolsulfosaeure

RN: 98-11-3 **MP** (°C)**:** 43
MW: 158.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.088E+00	4.885E+02	31.4	T023	1 2 2 1 2	
3.109E+00	4.917E+02	42.6	T023	1 2 2 1 2	
3.136E+00	4.960E+02	56.0	T023	1 2 2 1 2	
3.154E+00	4.989E+02	61.3	T023	1 2 2 1 2	

757. $C_6H_6O_3S.H_2O$

Benzenesulfonic acid (monohydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 176.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E+00	4.478E+02	21.3	T023	1 2 2 1 2	
2.568E+00	4.525E+02	31.0	T023	1 2 2 1 2	
2.770E+00	4.881E+02	32.6	T023	1 2 2 1 2	

(*continued*)

757. $C_6H_6O_3S.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.598E+00	4.577E+02	39.5	T023	1 2 2 1 2	
2.751E+00	4.846E+02	39.8	T023	1 2 2 1 2	
2.722E+00	4.796E+02	49.0	T023	1 2 2 1 2	
2.641E+00	4.654E+02	49.0	T023	1 2 2 1 2	
2.682E+00	4.726E+02	52.4	T023	1 2 2 1 2	

758. $C_6H_6O_3S.2.5H_2O$

Benzenesulfonic acid (2.5 hydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 203.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.281E+02	–4.0	T023	1 2 2 1 2	
2.122E+00	4.312E+02	–3.3	T023	1 2 2 1 2	
2.150E+00	4.370E+02	–2.3	T023	1 2 2 1 2	
2.131E+00	4.331E+02	–2.5	T023	1 2 2 1 2	

759. $C_6H_6O_3S.2H_2O$

Benzenesulfonic acid (dihydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E+00	4.370E+02	2.2	T023	1 2 2 1 2	
2.265E+00	4.399E+02	7.5	T023	1 2 2 1 2	
2.289E+00	4.446E+02	13.7	T023	1 2 2 1 2	
2.297E+00	4.460E+02	15.1	T023	1 2 2 1 2	

760. $C_6H_6O_3S.3H_2O$

Benzenesulfonic acid (trihydrate)

RN: 98-11-3 **MP** (°C)**:**
MW: 212.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E+00	3.586E+02	–40.8	T023	1 2 2 1 2	
1.766E+00	3.748E+02	–29.0	T023	1 2 2 1 2	
1.842E+00	3.909E+02	–18.5	T023	1 2 2 1 2	
1.922E+00	4.078E+02	–10.0	T023	1 2 2 1 2	
1.975E+00	4.191E+02	–5.9	T023	1 2 2 1 2	
2.011E+00	4.267E+02	–4.7	T023	1 2 2 1 2	

761. $C_6H_6O_4$
Muconic acid
Muconsaeure
RN: 505-70-4 **MP** (°C)**:**
MW: 142.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.407E-03	2.000E-01	20	F300	1 0 0 0 2	

762. $C_6H_7F_3N_4OS$
Thiazafluron
Urea, *N*,*N*′-dimethyl-*N*-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-
RN: 25366-23-8 **MP** (°C)**:** 136.5
MW: 240.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.724E-03	2.096E+00	20	E048	1 2 1 1 2	
8.742E-03	2.100E+00	20	M161	1 0 0 0 1	

763. C_6H_7N
Aniline
Aminobenzene
C.I. Oxidation base 1
Aminophen
Kyanol
RN: 62-53-3 **MP** (°C)**:** –6.3
MW: 93.13 **BP** (°C)**:** 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.531E-01	3.288E+01	8.60	C058	2 0 2 1 1	
3.877E-01	3.611E+01	13.8	K119	1 0 0 0 2	
3.747E-01	3.490E+01	18	F300	1 0 0 0 2	
3.818E-01	3.556E+01	18.15	P057	0 0 0 0 0	
3.612E-01	3.364E+01	22	H072	1 0 1 1 2	
3.930E-01	3.660E+01	22.5	G301	0 0 0 0 0	
3.931E-01	3.661E+01	25	B019	1 0 1 2 0	
3.931E-01	3.661E+01	25	B092	2 1 1 1 2	
4.000E-01	3.725E+01	25	F044	1 0 0 0 1	
3.791E-01	3.531E+01	25	G323	2 2 2 2 2	
3.800E-01	3.539E+01	25	H028	2 0 2 0 2	
3.791E-01	3.531E+01	25	H078	1 2 1 0 2	
3.650E-01	3.399E+01	25	M116	2 1 1 1 2	
3.731E-01	3.475E+01	25.40	C058	2 0 2 1 1	
3.930E-01	3.660E+01	26.70	L095	2 2 1 1 2	
4.229E-01	3.939E+01	48.00	C058	2 0 2 1 1	
4.328E-01	4.031E+01	50	G323	2 2 2 2 2	
5.016E-01	4.671E+01	60	B092	2 1 1 1 2	
5.016E-01	4.671E+01	66.30	C058	2 0 2 1 1	
7.025E-01	6.542E+01	96.70	C058	2 0 2 1 1	
3.801E-01	3.540E+01	ns	A406	0 0 0 0 1	

764. C_6H_7NO

m-Aminophenol
3-Aminophenol

RN: 591-27-5 **MP** (°C)**:** 125
MW: 109.13 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.797E-01	1.961E+01	10	M043	1 0 0 0 1	
2.291E-01	2.500E+01	20	F300	1 0 0 0 1	
2.409E-01	2.629E+01	20	M043	1 0 0 0 1	
3.355E-01	3.661E+01	30	M043	1 0 0 0 1	
3.261E-01	3.559E+01	32.6	S120	1 2 1 1 2	
4.859E-01	5.303E+01	40	M043	1 0 0 0 1	
6.788E-01	7.407E+01	47.9	S120	1 2 1 1 2	
8.850E-01	9.658E+01	53.0	S120	1 2 1 1 2	
1.590E+00	1.736E+02	60	M043	1 0 0 0 1	
1.406E+00	1.535E+02	60.4	S120	1 2 1 1 2	
2.148E+00	2.344E+02	66.4	S120	1 2 1 1 2	
2.627E+00	2.866E+02	68.9	S120	1 2 1 1 2	
2.927E+00	3.194E+02	70.2	S120	1 2 1 1 2	
3.161E+00	3.450E+02	71.5	S120	1 2 1 1 2	
3.410E+00	3.721E+02	73.2	S120	1 2 1 1 2	
3.737E+00	4.078E+02	77.2	S120	1 2 1 1 2	
6.752E+00	7.368E+02	80	M043	1 0 0 0 2	
4.098E+00	4.472E+02	85.2	S120	1 2 1 1 2	
4.311E+00	4.705E+02	96.0	S120	1 2 1 1 2	
8.291E+00	9.048E+02	100	M043	1 0 0 0 2	

765. C_6H_7NO

o-Aminophenol
2-Amino-phenol

RN: 95-55-6 **MP** (°C)**:** 172
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-01	1.700E+01	0	F300	1 0 0 0 1	
1.532E-01	1.672E+01	0	M043	1 0 0 0 1	
1.709E-01	1.865E+01	10	M043	1 0 0 0 1	
1.797E-01	1.961E+01	20	M043	1 0 0 0 1	
1.973E-01	2.153E+01	30	M043	1 0 0 0 1	
2.148E-01	2.344E+01	40	M043	1 0 0 0 1	
2.409E-01	2.629E+01	60	M043	1 0 0 0 1	
2.669E-01	2.913E+01	80	M043	1 0 0 0 1	
2.686E-01	2.931E+01	80.8	S120	1 2 1 1 1	
3.558E-01	3.883E+01	88.0	S120	1 2 1 1 1	
5.995E-01	6.542E+01	100	M043	1 0 0 0 1	

766. C_6H_7NO
p-Aminophenol
4-Aminophenol
RN: 123-30-8 **MP** (°C)**:** 190
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-01	1.100E+01	0	F300	1 0 0 0 1	
9.970E-02	1.088E+01	0	M043	1 0 0 0 1	
1.176E-01	1.283E+01	10	M043	1 0 0 0 1	
1.443E-01	1.575E+01	20	M043	1 0 0 0 1	
1.709E-01	1.865E+01	30	M043	1 0 0 0 1	
2.060E-01	2.248E+01	40	M043	1 0 0 0 1	
2.678E-01	2.922E+01	59.0	S120	1 2 1 1 1	
3.184E-01	3.475E+01	60	M043	1 0 0 0 1	
5.544E-01	6.050E+01	77.0	S120	1 2 1 1 1	
6.709E-01	7.322E+01	80	M043	1 0 0 0 1	
8.399E-01	9.165E+01	86.7	S120	1 2 1 1 1	
1.497E+00	1.634E+02	96.6	S120	1 2 1 1 1	
2.475E+00	2.701E+02	100	M043	1 0 0 0 1	

767. C_6H_7NO
Phenylhydroxylamine
Phenylhydroxylamin
RN: 100-65-2 **MP** (°C)**:** 82
MW: 109.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-01	2.000E+01	5	F300	1 0 0 0 0	
8.247E-01	9.000E+01	100	F300	1 0 0 0 0	

768. $C_6H_7NO_2S$
Benzenesulfonamide
Benzolsulfosaeure-amid
RN: 98-10-2 **MP** (°C)**:** 151
MW: 157.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	2.515E+00	15	K024	1 2 1 1 2	
2.736E-02	4.300E+00	16	F300	1 0 0 0 1	

769. $C_6H_7NO_3S$
Orthanilic acid
Orthanilsaeure
RN: 88-21-1 **MP** (°C)**:** 325
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.525E-02	1.130E+01	8.25	P038	1 1 2 1 2	monohydrate
7.535E-02	1.305E+01	12.3	P038	1 1 2 1 2	monohydrate
8.459E-02	1.465E+01	15.55	P038	1 1 2 1 2	anhydrate
8.776E-02	1.520E+01	16.75	P038	1 1 2 1 2	anhydrate
1.114E-01	1.930E+01	25	P038	1 1 2 1 2	anhydrate
1.738E-01	3.010E+01	41.3	P038	1 1 2 1 2	anhydrate
2.477E-01	4.290E+01	55.0	P038	1 1 2 1 2	anhydrate
3.672E-01	6.360E+01	70.0	P038	1 1 2 1 2	anhydrate
5.185E-01	8.980E+01	85.0	P038	1 1 2 1 2	anhydrate
4.585E-02	7.940E+00	.0	P038	1 1 2 1 2	monohydrate

770. $C_6H_7NO_3S$
Sulfanilic acid
4-Aminobenzenesulfonic acid
Sulfanilsaeure
RN: 121-57-3 **MP** (°C)**:** 122
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-02	6.359E+00	0	D077	1 0 0 1 1	
2.587E-02	4.480E+00	0	M043	1 0 0 0 1	
4.810E-02	8.330E+00	10	D077	1 0 0 1 1	
4.850E-02	8.400E+00	10	F300	1 0 0 0 1	
4.583E-02	7.937E+00	10	M043	1 0 0 0 1	
6.169E-02	1.068E+01	20	D077	1 0 0 1 2	
5.774E-02	1.000E+01	20	F300	1 0 0 0 1	
6.395E-02	1.108E+01	20	M043	1 0 0 0 2	
8.477E-02	1.468E+01	30	D077	1 0 0 1 2	
1.115E-01	1.932E+01	40	D077	1 0 0 1 2	
1.109E-01	1.920E+01	40	F300	1 0 0 0 2	
1.149E-01	1.990E+01	40	M043	1 0 0 0 2	
1.414E-01	2.449E+01	50	D077	1 0 0 1 2	
1.736E-01	3.007E+01	60	D077	1 0 0 1 2	
1.687E-01	2.922E+01	60	M043	1 0 0 0 2	
2.159E-01	3.740E+01	69.9	P038	1 0 2 1 2	anhydrate
2.103E-01	3.642E+01	70	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	M043	1 0 0 0 2	
2.737E-01	4.740E+01	85.0	P038	1 0 2 1 2	anhydrate
3.031E-01	5.249E+01	90	D077	1 0 0 1 2	
3.610E-01	6.253E+01	100	D077	1 0 0 1 2	
3.851E-01	6.670E+01	100	F300	1 0 0 0 2	
3.610E-01	6.253E+01	100	M043	1 0 0 0 2	
6.075E-02	1.052E+01	ns	K076	0 0 0 0 2	

771. $C_6H_7NO_3S$
Metanilic acid
3-Aminobenzenesulfonic acid
m-Sulfanilic acid
RN: 121-47-1 **MP** (°C)**:** >300
MW: 173.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.901E-02	1.022E+01	7.75	P038	1 2 2 1 2	anhydrate
7.622E-02	1.320E+01	16.75	P038	1 2 2 1 2	anhydrate
9.440E-02	1.635E+01	24.95	P038	1 2 2 1 2	anhydrate
1.383E-01	2.395E+01	40.0	P038	1 2 2 1 2	anhydrate
1.975E-01	3.420E+01	55.0	P038	1 2 2 1 2	anhydrate
2.714E-01	4.700E+01	70.0	P038	1 2 2 1 2	anhydrate
4.561E-02	7.900E+00	.0	P038	1 2 2 1 2	anhydrate

772. $C_6H_7NO_3S.1.5H_2O$
Metanilic acid (sesquihydrate)
3-Aminobenzenesulfonic acid (sesquihydrate)
RN: 121-47-1 **MP** (°C)**:**
MW: 200.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.041E-02	1.610E+01	8.35	P038	1 2 2 1 2	
1.119E-01	2.240E+01	15.55	P038	1 2 2 1 2	
1.184E-01	2.370E+01	16.8	P038	1 2 2 1 2	
3.247E-01	6.500E+01	85.0	P038	1 2 2 1 2	
5.344E-02	1.070E+01	.0	P038	1 2 2 1 2	

773. $C_6H_7NO_4S$
2-Aminophenol-4-sulfonic acid
2-Amino-phenol-sulfosaeure-(4)
RN: 98-37-3 **MP** (°C)**:** >300
MW: 189.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-02	1.000E+01	14	F300	1 0 0 0 0	

774. $C_6H_7NO_4S$
4-Aminophenol-2-sulfonic acid
4-Amino-phenol-sulfosaeure-(2)
RN: 2835-04-3 **MP** (°C)**:**
MW: 189.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	7.000E-01	14	F300	1 0 0 0 0	

775. $C_6H_7N_3O$
Isoniazid
Isonicotinic acid hydrazide
laniazid
RN: 54-85-3 **MP** (°C)**:** 171
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.813E-01	1.071E+02	20	I307	0 0 0 0 0	
8.955E-01	1.228E+02	25	B187	0 0 0 0 0	
1.458E+00	2.000E+02	37	I307	0 0 0 0 0	
1.505E+00	2.063E+02	40	B187	0 0 0 0 0	
9.115E-01	1.250E+02	ns	K444	0 0 0 0 0	

776. $C_6H_7N_3O_3$
Orotic acid methylamide
Orotamide, *N*-methyl-
RN: 1009-04-7 **MP** (°C)**:** 284–286
MW: 169.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.420E-01	5.785E+01	–4	N018	0 0 0 0 0	
6.840E-01	1.157E+02	16	N018	0 0 0 0 0	
8.340E-01	1.411E+02	25	N018	0 0 0 0 0	

777. $C_6H_7N_7$
2,4,7-Triaminopteridine
2:4:7-Triaminopteridine
RN: 14439-13-5 **MP** (°C)**:**
MW: 177.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.254E-03	2.222E-01	20	A020	1 2 0 0 1	
2.808E-02	4.975E+00	100	A020	1 2 0 0 0	

778. $C_6H_7N_7$
4,6,7-Triaminopteridine
4:6:7-Triaminopteridine
RN: 19167-62-5 **MP** (°C)**:**
MW: 177.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.515E-04	7.999E-02	20	A020	1 2 0 1 1	
1.252E-02	2.217E+00	100	A020	1 2 0 0 1	

779. $C_6H_7O_2P$
Phenylphosphinic acid
Phenyl-phosphinigsaeure
RN: 1779-48-2 **MP** (°C)**:** 84
MW: 142.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.757E-01	6.760E+01	14	F300	1 0 0 0 2	
9.460E+00	1.344E+03	24.63	W422	0 0 0 0 0	
1.109E+01	1.576E+03	27.09	W422	0 0 0 0 0	
1.294E+01	1.839E+03	29.24	W422	0 0 0 0 0	
1.593E+01	2.264E+03	32.06	W422	0 0 0 0 0	
2.177E+01	3.093E+03	36.77	W422	0 0 0 0 0	
3.047E+01	4.330E+03	39.68	W422	0 0 0 0 0	
4.843E+00	6.881E+02	100	F300	1 0 0 0 2	

780. $C_6H_7O_3P$
Phenylphosphonic acid
Phenylphosphonsaeure
RN: 1571-33-1 **MP** (°C)**:** 164.5
MW: 158.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.900E+02	15	F300	1 0 0 0 2	
1.202E+00	1.901E+02	ns	R427	0 0 0 0 0	

781. $C_6H_7O_3As$
Benzenearsonic acid
Phenylarsonsaeure
RN: 98-05-5 **MP** (°C)**:** 160
MW: 202.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.564E-01	3.160E+01	28	F300	1 0 0 0 2	
9.899E-01	2.000E+02	84	F300	1 0 0 0 1	

782. C_6H_8
1,4-Cyclohexadiene
1,4-Dihydrobenzene
RN: 628-41-1 **MP** (°C)**:** –49.2
MW: 80.13 **BP** (°C)**:** 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-02	8.512E-01	4.8	L007	2 2 1 2 2	
1.062E-02	8.512E-01	5.1	L007	2 1 1 1 2	
1.195E-02	9.576E-01	14.8	L007	2 2 1 2 2	

(*continued*)

782. C_6H_8 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-02	9.576E-01	15.2	L007	2 1 1 1 2	
8.002E-03	6.412E-01	20	M337	2 1 2 2 2	
1.167E-02	9.353E-01	24.8	L007	2 2 1 2 2	
8.736E-03	7.000E-01	25	M001	2 1 2 2 2	
1.167E-02	9.353E-01	25.1	L007	2 1 1 1 2	
1.201E-02	9.625E-01	34.8	L007	2 2 1 2 2	
1.201E-02	9.625E-01	35.2	L007	2 1 1 1 2	
1.259E-02	1.009E+00	44.8	L007	2 2 1 2 2	
1.259E-02	1.009E+00	45.2	L007	2 1 1 1 2	

783. $C_6H_8ClN_7O$
Amiloride
RN: 2609-46-3 **MP** (°C)**:**
MW: 229.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.531E-04	1.500E-01	22.5	B422	0 0 0 0 0	
2.870E+00	6.590E+02	25	B443	0 0 0 0 0	

784. $C_6H_8N_2$
2,5-Dimethylpyrazine
2,5-Dimethyl-pyrazin
RN: 123-32-0 **MP** (°C)**:** 63
MW: 108.14 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		25	D425	0 0 0 0 0	

785. $C_6H_8N_2$
m-Phenylenediamine
m-Phenylendiamin
RN: 108-45-2 **MP** (°C)**:** 63
MW: 108.14 **BP** (°C)**:** 283

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.409E-01	8.012E+01	.3	S115	1 2 1 1 2	α form
2.928E-01	3.166E+01	.3	S115	1 2 1 1 2	β form
1.038E+00	1.122E+02	4.6	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	9.3	S115	1 2 1 1 2	α form
1.618E+00	1.750E+02	11.7	S115	1 2 1 1 2	α form
7.806E-01	8.442E+01	14.3	S115	1 2 1 1 2	β form
2.285E+00	2.472E+02	16.1	S115	1 2 1 1 2	α form
2.671E+00	2.889E+02	17.3	S115	1 2 1 1 2	α form
1.038E+00	1.122E+02	18.3	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	18.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	19.9	S115	1 2 1 1 2	α form

(*continued*)

785. $C_6H_8N_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.537E+00	3.825E+02	20.8	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	22.0	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	22.7	S115	1 2 1 1 2	α form
1.480E+00	1.600E+02	23.1	S115	1 2 1 1 2	β form
1.618E+00	1.750E+02	24.1	S115	1 2 1 1 2	β form
1.918E+00	2.074E+02	25.1	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	26.0	S115	1 2 1 1 2	α form
2.285E+00	2.472E+02	26.3	S115	1 2 1 1 2	β form
2.671E+00	2.889E+02	27.1	S115	1 2 1 1 2	β form
2.815E+00	3.044E+02	27.1	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	27.9	S115	1 2 1 1 2	β form
4.085E+00	4.418E+02	28.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	29.0	S115	1 2 1 1 2	β form
3.537E+00	3.825E+02	29.1	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	30.2	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	31.5	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	32.6	S115	1 2 1 1 2	α form
4.085E+00	4.418E+02	32.8	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	34.4	S115	1 2 1 1 2	β form
4.439E+00	4.800E+02	43.5	S115	1 2 1 1 2	α form
4.549E+00	4.919E+02	53.6	S115	1 2 1 1 2	α form
4.586E+00	4.960E+02	57.6	S115	1 2 1 1 2	α form
4.623E+00	5.000E+02	62.8	S115	1 2 1 1 2	α form

786. $C_6H_8N_2$

o-Phenylenediamine
o-Phenylendiamin

RN: 95-54-5 **MP** (°C)**:** 102–103
MW: 108.14 **BP** (°C)**:** 257

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.876E-01	3.110E+01	20	T301	1 2 2 2 2	
3.763E-01	4.070E+01	35	F300	1 0 0 0 2	
3.599E-01	3.892E+01	35.1	S115	1 2 1 1 2	
5.110E-01	5.527E+01	45.8	S115	1 2 1 1 2	
9.804E-01	1.060E+02	56.3	S115	1 2 1 1 2	
1.458E+00	1.577E+02	61.3	S115	1 2 1 1 2	
1.755E+00	1.898E+02	62.8	S115	1 2 1 1 2	
2.218E+00	2.398E+02	64.2	S115	1 2 1 1 2	
2.948E+00	3.188E+02	66.1	S115	1 2 1 1 2	
3.558E+00	3.847E+02	67.7	S115	1 2 1 1 2	
3.955E+00	4.277E+02	71.3	S115	1 2 1 1 2	
4.338E+00	4.691E+02	80.8	S115	1 2 1 1 2	
4.476E+00	4.841E+02	88.1	S115	1 2 1 1 2	
4.533E+00	4.902E+02	91.7	S115	1 2 1 1 2	
4.570E+00	4.942E+02	95.5	S115	1 2 1 1 2	

787. $C_6H_8N_2$
p-Phenylenediamine
1,4-Phenylenediamine
RN: 106-50-3 **MP** (°C)**:** 141
MW: 108.14 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.880E-02	1.068E+01	3.6	S115	1 2 1 1 2	
3.299E-01	3.568E+01	23.7	S115	1 2 1 1 2	
4.180E-01	4.520E+01	25	F300	1 0 0 0 2	
8.292E-01	8.967E+01	37.8	S115	1 2 1 1 2	
1.460E+00	1.579E+02	49.9	S115	1 2 1 1 2	
1.978E+00	2.140E+02	59.2	S115	1 2 1 1 2	
2.368E+00	2.561E+02	64.6	S115	1 2 1 1 2	
2.724E+00	2.945E+02	69.2	S115	1 2 1 1 2	
3.155E+00	3.412E+02	75.5	S115	1 2 1 1 2	
3.432E+00	3.711E+02	80.3	S115	1 2 1 1 2	
3.809E+00	4.119E+02	88.5	S115	1 2 1 1 2	
4.055E+00	4.385E+02	95.9	S115	1 2 1 1 2	
1.500E-05	1.622E-03	98.59	M180	0 0 2 2 0	EFG
2.500E-05	2.704E-03	111.46	M180	0 0 2 2 0	EFG
4.000E-05	4.326E-03	117.47	M180	0 0 2 2 0	EFG
4.500E-05	4.866E-03	122.10	M180	0 0 2 2 0	EFG
5.000E-05	5.407E-03	126.84	M180	0 0 2 2 0	EFG
7.000E-05	7.570E-03	133.34	M180	0 0 2 2 0	EFG

788. $C_6H_8N_2OS$
5,6-Dimethyl-2-thiouracil
4(1H)-Pyrimidinone, 2,3-dihydro-5,6-dimethyl-2-thioxo-
5,6-Dimethylthiouracil
RN: 28456-54-4 **MP** (°C)**:**
MW: 156.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.790E-03	1.373E+00	25	G016	1 2 1 2 2	intrinsic

789. $C_6H_8N_2O_2$
N,N-1,3-Dimethyluracil
1,3-Dimethyl-2,4-pyrimidinedione
*N*1,*N*3-Dimethyluracil
N,N′-Dimethyluracil
1,3-Dimethyluracil
RN: 874-14-6 **MP** (°C)**:**
MW: 140.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.568E+00	5.000E+02	ns	B177	0 0 0 0 2	

790. $C_6H_8N_2O_2S$
o-Aminobenzenesulfonamide
Orthanilamide
RN: 3306-62-5 **MP** (°C)**:**
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-02	6.458E+00	23	K034	2 2 2 2 1	
3.865E-02	6.655E+00	24	K034	2 2 2 2 1	
4.323E-02	7.444E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	28	K034	2 2 2 2 1	
5.237E-02	9.018E+00	30.5	K034	2 2 2 2 1	
5.806E-02	9.999E+00	33	K034	2 2 2 2 2	
6.034E-02	1.039E+01	34	K034	2 2 2 2 2	
6.375E-02	1.098E+01	35.5	K034	2 2 2 2 2	
6.886E-02	1.186E+01	37	K034	2 2 2 2 2	
6.829E-02	1.176E+01	37	K034	2 2 2 2 2	
8.356E-02	1.439E+01	42	K034	2 2 2 2 2	
9.707E-02	1.672E+01	46	K034	2 2 2 2 2	
1.139E-01	1.961E+01	50	K034	2 2 2 2 2	

791. $C_6H_8N_2O_2S$
m-Aminobenzenesulfonamide
Metanilamide
m-Amidobenzenesulfonamide
RN: 98-18-0 **MP** (°C)**:**
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.545E-02	1.127E+01	23	K034	2 2 2 2 2	
6.942E-02	1.196E+01	24	K034	2 2 2 2 2	
7.678E-02	1.322E+01	26	K034	2 2 2 2 2	
8.469E-02	1.458E+01	28	K034	2 2 2 2 2	
1.077E-01	1.855E+01	33	K034	2 2 2 2 2	
1.244E-01	2.143E+01	35.5	K034	2 2 2 2 2	
1.339E-01	2.306E+01	37	K034	2 2 2 2 2	
1.461E-01	2.515E+01	39	K034	2 2 2 2 2	
1.697E-01	2.922E+01	42	K034	2 2 2 2 2	
2.072E-01	3.568E+01	46	K034	2 2 2 2 2	
2.543E-01	4.379E+01	50	K034	2 2 2 2 2	

792. $C_6H_8N_2O_2S$

Benzenesulfamide
Sulfanilamide
Sulfanilsaeure-amid
p-Aminobenzenesulphonamide

RN: 63-74-1 **MP** (°C)**:** 165
MW: 172.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	1	A047	1 0 0 0 0	EFG
1.057E-02	1.820E+00	4.40	B147	1 2 1 1 2	
1.458E-02	2.510E+00	10.20	B147	1 2 1 1 2	
1.957E-02	3.370E+00	15	B147	1 2 1 1 2	
2.323E-02	4.000E+00	15	F300	1 0 0 0 0	
2.660E-02	4.581E+00	15	K024	1 2 1 1 2	
2.241E-02	3.860E+00	15	S147	1 2 2 2 2	hydrate
2.889E-02	4.975E+00	16	A047	1 0 0 0 0	EFG
2.439E-02	4.200E+00	16	H114	1 0 0 0 2	
2.700E-02	4.650E+00	20	B147	1 2 1 1 2	
3.463E-02	5.964E+00	20	D041	1 0 0 0 0	
4.149E-02	7.145E+00	20	F073	1 2 2 2 2	
2.903E-02	5.000E+00	20	F300	1 0 0 0 0	
3.020E-02	5.200E+00	20	S147	1 2 2 2 2	hydrate
3.693E-02	6.359E+00	23	K034	2 2 2 2 1	
3.979E-02	6.853E+00	24	K034	2 2 2 2 1	
3.484E-02	6.000E+00	25	B147	1 2 1 1 2	
4.855E-02	8.360E+00	25	C102	2 0 2 2 2	
4.550E-02	7.835E+00	25	M116	2 1 1 1 2	
4.274E-02	7.360E+00	25	M440	0 0 0 0 0	
4.820E-02	8.300E+00	25	P015	0 0 0 0 0	
4.216E-02	7.260E+00	25	S147	1 2 2 2 2	hydrate
4.437E-02	7.641E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	27	K034	2 2 2 2 1	
5.008E-02	8.625E+00	28	K034	2 2 2 2 1	
4.762E-02	8.200E+00	30	B147	1 2 1 1 2	
5.633E-02	9.700E+00	30	S147	1 2 2 2 2	hydrate
5.806E-02	9.999E+00	30.5	K034	2 2 2 2 2	
6.318E-02	1.088E+01	31	A047	1 0 0 0 0	EFG
6.205E-02	1.068E+01	31.7	K034	2 2 2 2 2	
6.829E-02	1.176E+01	33	K034	2 2 2 2 2	
7.282E-02	1.254E+01	34	K034	2 2 2 2 2	
6.388E-02	1.100E+01	35	B147	1 2 1 1 2	
7.543E-02	1.299E+01	35	S147	1 2 2 2 2	β form
7.848E-02	1.351E+01	35.5	K034	2 2 2 2 2	
1.259E-01	2.168E+01	37	A028	1 0 2 1 2	intrinsic
7.375E-02	1.270E+01	37	B147	1 2 1 1 2	
8.478E-02	1.460E+01	37	C102	2 0 2 2 2	
8.594E-02	1.480E+01	37	D084	1 0 1 0 2	
8.018E-02	1.381E+01	37	F072	1 0 0 0 2	
8.710E-02	1.500E+01	37	F300	1 0 0 0 1	
8.920E-02	1.536E+01	37	G028	2 2 1 1 2	δ form, recrystallized

(*continued*)

792. $C_6H_8N_2O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.070E-02	1.562E+01	37	G028	2 2 1 1 2	β form, recrystallized
9.120E-02	1.571E+01	37	G028	2 2 1 1 2	α form, recrystallized
9.240E-02	1.591E+01	37	G028	2 2 1 1 2	γ form
8.413E-02	1.449E+01	37	K034	2 2 2 2 2	
8.652E-02	1.490E+01	37	K086	1 0 0 0 2	
8.210E-02	1.414E+01	37	K095	2 0 0 0 2	intrinsic
8.710E-02	1.500E+01	37	L091	1 0 0 0 2	pH 5.5
8.469E-02	1.458E+01	37.50	M142	1 0 0 0 2	
9.201E-02	1.584E+01	39	K034	2 2 2 2 2	
8.362E-02	1.440E+01	40	B147	1 2 1 1 2	form II
9.750E-02	1.679E+01	40	G028	2 2 1 1 2	α form, recrystallized
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	γ form
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	δ form, recrystallized
9.680E-02	1.667E+01	40	G028	2 2 1 1 2	β form, recrystallized
9.518E-02	1.639E+01	40	S147	1 2 2 2 2	β form
1.049E-01	1.807E+01	42	K034	2 2 2 2 2	
1.086E-01	1.870E+01	45	B147	1 2 1 1 2	form II
1.201E-01	2.069E+01	45	S147	1 2 2 2 2	β form
1.256E-01	2.162E+01	46	K034	2 2 2 2 2	
1.527E-01	2.629E+01	50	A047	1 0 0 0 0	EFG
1.388E-01	2.390E+01	50	B147	1 2 1 1 2	form II
1.433E-01	2.468E+01	50	G028	2 2 1 1 2	δ form, recrystallized
1.419E-01	2.444E+01	50	G028	2 2 1 1 2	β form, recrystallized
1.430E-01	2.463E+01	50	G028	2 2 1 1 2	γ form
1.435E-01	2.471E+01	50	G028	2 2 1 1 2	α form, recrystallized
1.516E-01	2.610E+01	50	K034	2 2 2 2 2	
1.488E-01	2.562E+01	50	S147	1 2 2 2 2	β form
1.789E-01	3.080E+01	55	B147	1 2 1 1 2	form II
2.294E-01	3.950E+01	60	B147	1 2 1 1 2	form II
2.923E-01	5.033E+01	65	A047	1 0 0 0 0	EFG
2.962E-01	5.100E+01	65	B147	1 2 1 1 2	form II
3.833E-01	6.600E+01	70	B147	1 2 1 1 2	form II
4.599E-01	7.919E+01	75	A047	1 0 0 0 0	EFG
5.168E-01	8.900E+01	75	B147	1 2 1 1 2	form II
5.660E-01	9.747E+01	79	A047	1 0 0 0 0	EFG
6.272E-02	1.080E+01	ns	D035	0 0 0 0 2	
3.050E-02	5.252E+00	ns	L044	0 0 0 0 2	
4.571E-02	7.871E+00	ns	R427	0 0 0 0 0	
4.365E-02	7.517E+00	ns	R428	0 0 0 0 0	

793. $C_6H_8N_2O_2S.H_2O$
Sulfanilamide (monohydrate)
4-Aminobenzenesulfonamide (monohydrate)
p-Anilinesulfonamide (monohydrate)
Bacteramid (monohydrate)
RN: 20203-81-0 **MP** (°C)**:**
MW: 190.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	4.185E+00	15	G028	2 2 1 1 2	
4.320E-02	8.218E+00	26	G028	2 2 1 1 2	
5.600E-02	1.065E+01	30	G028	2 2 1 1 2	
8.420E-02	1.602E+01	37	G028	2 2 1 1 2	

794. $C_6H_8N_2O_3$
5,5-Dimethylbarbituric acid
5,5-Dimethylbarbitursaeure
Barbituric acid, 5,5-dimethyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-dimethyl
5,5-Dimethyl barbituric acid
5,5-Dimethylbarbiturate
RN: 24448-94-0 **MP** (°C)**:** 278
MW: 156.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.812E-02	2.829E+00	25	P350	0 0 0 0 0	intrinsic
1.549E-02	2.419E+00	ns	T003	0 0 0 0 2	

795. $C_6H_8N_2O_3S$
4-Phenylhydrazine sulfonic acid
Phenylhydrazin-sulfosaeure-(4)
RN: 98-71-5 **MP** (°C)**:**
MW: 188.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.029E-02	5.700E+00	11.50	F300	1 0 0 0 1	
1.860E-01	3.500E+01	100	F300	1 0 0 0 1	

796. $C_6H_8N_2O_8$
Isosorbide dinitrate
1,4:3,6-Dianhydro-D-glucitol dinitrate
Sorbidin
Isogen
Imdur
RN: 87-33-2 **MP** (°C)**:** 70
MW: 236.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-03	5.497E-01	25	L033	1 0 2 1 2	

797. $C_6H_8N_4O$
5-Amino-4-carboxymethylaminopyrimidine
RN: **MP** (°C)**:**
MW: 152.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-01	3.226E+01	100	A082	1 2 0 0 0	

798. $C_6H_8N_8$
2,4,6,7-Tetraminopteridine
2:4:6:7-Tetraminopteridine
RN: 19167-63-6 **MP** (°C)**:**
MW: 192.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.002E-04	7.692E-02	20	A020	1 2 0 1 1	

799. $C_6H_8O_2$
Sorbic acid
2,4-Hexadienoic acid
2-Propenylacrylic acid
Preservastat
Hexadienoic acid
Sorbistat
RN: 110-44-1 **MP** (°C)**:** 134.5
MW: 112.13 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	1.906E+00	30	L069	1 0 1 1 0	EFG

800. $C_6H_8O_6$
Tricarballylic acid
Tricarballylsaeure
1,2,3-Propanetricarboxylic acid
RN: 99-14-9 **MP** (°C)**:** 166
MW: 176.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.885E+00	3.320E+02	18	F300	1 0 0 0 2	

801. $C_6H_8O_6$
Ascorbic acid
L-Ascorbic acid
L-Ascorbinsaeure
RN: 50-81-7 **MP** (°C)**:** 193
MW: 176.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.269E-01	1.633E+02	6.99	A341	0 0 0 0 0	
9.509E-01	1.675E+02	7.99	A341	0 0 0 0 0	
9.880E-01	1.740E+02	9.99	A341	0 0 0 0 0	
1.026E+00	1.807E+02	11.99	A341	0 0 0 0 0	
1.142E+00	2.011E+02	15.99	A341	0 0 0 0 0	
1.418E+00	2.498E+02	20	D041	1 0 0 0 2	
1.254E+00	2.208E+02	20	S472	0 0 0 0 0	
1.283E+00	2.260E+02	20.99	A341	0 0 0 0 0	
1.397E+00	2.460E+02	24.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	25	D315	0 0 0 0 0	
9.757E-01	1.718E+02	25	N003	0 0 0 0 0	
1.388E+00	2.445E+02	25	S472	0 0 0 0 0	
1.551E+00	2.731E+02	28.99	A341	0 0 0 0 0	
1.533E+00	2.699E+02	30	S472	0 0 0 0 0	
1.718E+00	3.025E+02	33.99	A341	0 0 0 0 0	
1.703E+00	2.999E+02	35	S472	0 0 0 0 0	
1.758E+00	3.096E+02	35.99	A341	0 0 0 0 0	
1.856E+00	3.270E+02	38.99	A341	0 0 0 0 0	
1.028E+00	1.810E+02	40	N003	0 0 0 0 0	
1.874E+00	3.301E+02	40	S472	0 0 0 0 0	
2.009E+00	3.539E+02	42.99	A341	0 0 0 0 0	
2.021E+00	3.560E+02	43.99	A341	0 0 0 0 0	
2.066E+00	3.638E+02	44.99	A341	0 0 0 0 0	
2.054E+00	3.618E+02	45	S472	0 0 0 0 0	
2.132E+00	3.755E+02	47.69	A341	0 0 0 0 0	
2.184E+00	3.847E+02	48.49	A341	0 0 0 0 0	
2.235E+00	3.937E+02	49.99	A341	0 0 0 0 0	
2.235E+00	3.936E+02	50	S472	0 0 0 0 0	
2.255E+00	3.972E+02	50.39	A341	0 0 0 0 0	
2.275E+00	4.007E+02	50.99	A341	0 0 0 0 0	
2.373E+00	4.180E+02	52.49	A341	0 0 0 0 0	

(*continued*)

801. $C_6H_8O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.383E+00	4.197E+02	53.99	A341	0 0 0 0 0	
2.413E+00	4.249E+02	54.09	A341	0 0 0 0 0	
2.449E+00	4.314E+02	54.99	A341	0 0 0 0 0	
2.520E+00	4.439E+02	60.02	A341	0 0 0 0 0	
2.551E+00	4.492E+02	61.99	A341	0 0 0 0 0	
2.635E+00	4.641E+02	64.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	ns	M054	0 0 0 0 2	

802. $C_6H_8O_7$

Citric acid anhydrous
2-Hydroxytricarballylic acid
Citronensaeure
1,2,3-Propanetricarboxylic acid
Citro
Citralite

RN: 77-92-9 **MP** (°C)**:** 153
MW: 192.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E+00	4.898E+02	0	M043	1 0 0 0 1	
1.881E+00	3.613E+02	1.2	K084	1 0 1 0 2	
1.875E+00	3.602E+02	1.6	K084	1 0 1 0 2	
2.562E+00	4.923E+02	4.99	A339	0 0 0 0 0	
1.825E+00	3.506E+02	10	D020	1 2 1 1 2	
2.571E+00	4.940E+02	10	F300	1 0 0 0 2	
1.825E+00	3.506E+02	10	F302	1 0 0 0 1	
2.817E+00	5.413E+02	10	M043	1 0 0 0 2	
1.938E+00	3.723E+02	10.0	K084	1 0 1 0 2	
2.684E+00	5.157E+02	9.99	A339	0 0 0 0 0	
1.927E+00	3.702E+02	10.8	K084	1 0 1 0 2	
2.811E+00	5.400E+02	14.99	A339	0 0 0 0 0	
1.933E+00	3.713E+02	15.0	K084	1 0 1 0 2	
2.918E+00	5.605E+02	19.99	A339	0 0 0 0 0	
3.089E+00	5.935E+02	20	D041	1 0 0 0 2	
2.816E+00	5.410E+02	20	F300	1 0 0 0 2	
1.935E+00	3.719E+02	20	F302	1 0 0 0 2	
3.089E+00	5.935E+02	20	M043	1 0 0 0 2	
3.045E+00	5.851E+02	24.99	A339	0 0 0 0 0	
1.994E+00	3.831E+02	25	D020	1 2 1 1 2	
1.254E+01	2.409E+03	25	K040	1 0 2 1 2	
3.201E+00	6.149E+02	29.99	A339	0 0 0 0 0	
2.037E+00	3.914E+02	30	F302	1 0 0 0 2	
3.366E+00	6.466E+02	30	M043	1 0 0 0 2	
3.296E+00	6.332E+02	34.99	A339	0 0 0 0 0	
2.100E+00	4.034E+02	35.8	D039	2 2 1 2 2	EFG
2.094E+00	4.023E+02	36.6	F302	1 0 0 0 2	
3.201E+00	6.150E+02	36.60	F300	1 0 0 0 2	

(*continued*)

802. $C_6H_8O_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.346E+00	6.429E+02	39.99	A339	0 0 0 0 0	
2.118E+00	4.069E+02	40	D020	1 2 1 1 2	
2.116E+00	4.065E+02	40	D039	2 2 1 2 0	EFG
2.118E+00	4.069E+02	40	F302	1 0 0 0 2	
3.553E+00	6.825E+02	40	M043	1 0 0 0 2	
3.438E+00	6.605E+02	44.99	A339	0 0 0 0 0	
3.488E+00	6.702E+02	49.99	A339	0 0 0 0 0	
2.161E+00	4.152E+02	50	D039	2 2 1 2 0	EFG
2.159E+00	4.149E+02	50	F302	1 0 0 0 2	
3.539E+00	6.800E+02	54.99	A339	0 0 0 0 0	
3.601E+00	6.918E+02	59.99	A339	0 0 0 0 0	
2.214E+00	4.253E+02	60	D039	2 2 1 2 0	EFG
2.205E+00	4.236E+02	60	F302	1 0 0 0 2	
3.824E+00	7.347E+02	60	M043	1 0 0 0 2	
3.669E+00	7.050E+02	64.99	A339	0 0 0 0 0	
2.261E+00	4.344E+02	70	D039	2 2 1 2 0	EFG
2.251E+00	4.325E+02	70	F302	1 0 0 0 2	
2.300E+00	4.420E+02	80	D039	2 2 1 2 0	EFG
2.294E+00	4.407E+02	80	F302	1 0 0 0 2	
4.102E+00	7.881E+02	80	M043	1 0 0 0 2	
2.350E+00	4.515E+02	90	D039	2 2 1 2 0	EFG
2.336E+00	4.487E+02	90	F302	1 0 0 0 2	
2.391E+00	4.595E+02	100	D039	2 2 1 2 0	EFG
4.372E+00	8.400E+02	100	D041	1 0 0 0 2	
3.997E+00	7.680E+02	100	F300	1 0 0 0 2	
2.376E+00	4.565E+02	100	F302	1 0 0 0 1	
4.373E+00	8.403E+02	100	M043	1 0 0 0 2	
1.885E+00	3.621E+02	.0	K084	1 0 1 0 2	

803. $C_6H_8O_7.H_2O$

Citric acid (monohydrate)
2-Hydroxytricarballylic acid (monohydrate)
RN: 5949-29-1 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E+00	3.266E+02	0	D039	2 2 1 2 0	EFG
1.667E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
3.005E+00	6.314E+02	17.20	L031	1 1 2 1 2	average of 2
3.077E+00	6.466E+02	19.80	L031	1 1 2 1 2	
1.771E+00	3.723E+02	20	D039	2 2 1 2 0	EFG
3.080E+00	6.473E+02	20.20	L031	1 1 2 1 2	
3.146E+00	6.610E+02	22.50	L031	1 1 2 1 2	
3.154E+00	6.627E+02	22.90	L031	1 1 2 1 2	
1.822E+00	3.830E+02	25	D039	2 2 1 2 2	EFG
3.214E+00	6.753E+02	25.10	L031	1 1 2 1 2	
3.216E+00	6.759E+02	25.30	L031	1 1 2 1 2	

(*continued*)

803. $C_6H_8O_7.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.272E+00	6.875E+02	27.00	L031	1 1 2 1 2	
3.276E+00	6.885E+02	27.60	L031	1 1 2 1 2	
3.303E+00	6.942E+02	28.60	L031	1 1 2 1 2	
1.864E+00	3.917E+02	30	D039	2 2 1 2 0	EFG
3.359E+00	7.059E+02	30.50	L031	1 1 2 1 2	
3.357E+00	7.054E+02	30.70	L031	1 1 2 1 2	
3.389E+00	7.122E+02	31.80	L031	1 1 2 1 2	
3.440E+00	7.230E+02	33.70	L031	1 1 2 1 2	
3.478E+00	7.308E+02	34.40	L031	1 1 2 1 2	
3.518E+00	7.392E+02	35.40	L031	1 1 2 1 2	

804. C_6H_8S

2-Ethylthiophene

Thiophene, 2-ethyl-

RN: 872-55-9 **MP** (°C)**:** <25

MW: 112.19 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.603E-03	2.920E-01	25	K119	1 0 0 0 2	
2.603E-03	2.920E-01	25	P051	2 1 1 2 2	
2.603E-03	2.920E-01	25.00	P007	2 1 2 2 2	

805. $C_6H_9ClO_3$

Ethyl 2-chloroacetoacetate

2-Chloroacetoacetic acid ethyl ester

RN: 609-15-4 **MP** (°C)**:**

MW: 164.59 **BP** (°C)**:** 107 at 14 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-02	8.900E+00	30	B433	0 0 0 0 0	

806. $C_6H_9NO_3$

4,6,10-Trioxa-1-azatricyclo[3.3.1.13,7]decane

Trimorpholin

Trimorpholine

RN: 281-36-7 **MP** (°C)**:**

MW: 143.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	1.670E+02	0	F300	1 0 0 0 2	
2.375E+00	3.400E+02	80	F300	1 0 0 0 2	

807. $C_6H_9NO_3$
Trimethadione
3,5,5-Trimethyl-2,4-diketooxazolidine
3,5,5-Trimethyl-2,4-oxazolidinedione
Tridione
RN: 127-48-0 **MP** (°C)**:** 46
MW: 143.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-01	4.762E+01	20	D041	1 0 0 0 0	

808. $C_6H_9NO_6$
Triglycine
Complexon I
N,N-bis(Carboxymethyl)glycine
α,α′,α²-Trimethylaminetricarboxylic acid
RN: 139-13-9 **MP** (°C)**:** 241.5
MW: 191.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-01	5.906E+01	25	M024	1 2 0 1 2	
3.395E-01	6.490E+01	25.1	N024	0 0 0 0 0	
3.374E-01	6.450E+01	25.1	N025	0 0 0 0 0	
3.348E-01	6.400E+01	25.1	N026	0 0 0 0 0	
3.101E-01	5.927E+01	25.1	N027	1 2 2 2 2	

809. $C_6H_9N_3$
Kyanmethin
6-Amino-2,4-dimethyl-pyrimidin
6-Amino-2,4-dimethylpyrimidine
RN: 461-98-3 **MP** (°C)**:** 182
MW: 123.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.197E-02	6.400E+00	18	F300	1 0 0 0 1	

810. $C_6H_9N_3O_2$
2-Isopropyl-4(5)-nitroimidazole
1H-Imidazole, 2-(1-methylethyl)-4-nitro-
2-(1-Methylethyl)-4-nitro-1H-imidazole
2-Isopropyl-5-nitroimidazole
2-Isopropyl-4-nitroimidazole
RN: 13373-32-5 **MP** (°C)**:** 182–183
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
6.886E-02	1.068E+01	20	D344	0 0 0 0 0	
7.030E-02	1.091E+01	20	D344	0 0 0 0 0	

811. $C_6H_9N_3O_2$
L-Histidine
L-Histidin
Histidine
RN: 71-00-1 **MP** (°C)**:** 287
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.580E-01	4.003E+01	15	D349	2 1 1 2 2	
2.646E-01	4.106E+01	20	B032	1 2 2 1 2	
2.640E-01	4.096E+01	20	D349	2 1 1 2 2	
2.930E-01	4.546E+01	25	B032	1 2 2 1 2	
2.574E-01	3.994E+01	25	D041	1 0 0 0 2	
2.720E-01	4.220E+01	25	D349	2 1 1 2 2	
2.481E-01	3.850E+01	25	F300	1 0 0 0 2	
2.651E-01	4.114E+01	25	G315	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N024	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N025	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N026	0 0 0 0 0	
2.675E-01	4.150E+01	25.1	N027	1 1 2 2 2	
2.791E-01	4.330E+01	27	D036	0 0 0 0 0	
3.207E-01	4.976E+01	29.80	B032	1 2 2 1 2	
2.834E-01	4.398E+01	30	H062	2 2 2 0 1	EFG
5.213E-01	8.088E+01	50	H062	2 2 2 0 0	EFG
7.915E-01	1.228E+02	70	H062	2 2 2 0 0	EFG

812. $C_6H_9N_3O_2$
6-Amino-1,3-dimethyluracil
RN: 6642-31-5 **MP** (°C)**:**
MW: 155.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.550E-02	7.060E+00	25	Z408	0 0 0 0 0	

813. $C_6H_9N_3O_3$
Metronidazole
Flagyl
2-Methyl-5-nitroimidazole-1-ethanol
Metrozine
Rozex
2-Methyl-5-nitro-1-imidazoleethanol
RN: 443-48-1 **MP** (°C)**:** 158
MW: 171.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.441E-02	9.312E+00	20	D344	0 0 0 0 0	
5.540E-02	9.482E+00	20	D344	0 0 0 0 0	
4.809E-02	8.232E+00	20	H324	0 0 0 0 0	
5.785E-02	9.901E+00	20	I315	0 0 0 0 0	
6.427E-02	1.100E+01	25	C062	1 1 2 1 2	
5.550E-02	9.500E+00	25	C124	2 0 1 1 2	
5.727E-02	9.803E+00	26	H324	0 0 0 0 0	
6.585E-02	1.127E+01	30	H324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	C324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	K444	0 0 0 0 0	

814. C_6H_{10}
1,5-Hexadiene
Biallyl
Diallyl
RN: 592-42-7 **MP** (°C)**:** –141
MW: 82.15 **BP** (°C)**:** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.057E-03	1.690E-01	25	M001	2 1 2 2 2	

815. C_6H_{10}
Cyclohexene
1,2,3,4-Tetrahydrobenzene
RN: 110-83-8 **MP** (°C)**:** –104
MW: 82.15 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-03	2.799E-01	4.8	L007	2 2 1 2 2	
3.408E-03	2.799E-01	5.1	L007	2 0 1 1 2	
3.633E-03	2.984E-01	14.8	L007	2 2 1 2 2	
3.633E-03	2.984E-01	15.2	L007	2 0 1 1 2	
1.583E-03	1.300E-01	20	C008	1 2 2 0 1	
2.769E-03	2.274E-01	20	M337	2 1 2 2 2	

(*continued*)

815. C_6H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-03	2.834E-01	23.5	S171	2 1 2 2 2	
3.639E-03	2.989E-01	24.8	L007	2 2 1 2 2	
2.593E-03	2.130E-01	25	M001	2 1 2 2 2	
3.639E-03	2.989E-01	25.1	L007	2 0 1 1 2	
3.681E-03	3.024E-01	34.8	L007	2 2 1 2 2	
3.681E-03	3.024E-01	35.2	L007	2 0 1 1 2	
6.000E-03	4.929E-01	40	P335	0 0 0 0 0	
3.779E-03	3.104E-01	44.8	L007	2 2 1 2 2	
3.779E-03	3.104E-01	45.2	L007	2 0 1 1 2	
1.800E-02	1.479E+00	140	P335	0 0 0 0 0	
1.583E-03	1.300E-01	ns	M010	0 0 0 0 1	

816. C_6H_{10}

1-Hexyne
Butylacetylene
n-Butylacetylene

RN: 693-02-7 **MP** (°C)**:** –132
MW: 82.15 **BP** (°C)**:** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.382E-03	3.600E-01	25	M001	2 1 2 2 2	
8.370E-03	6.876E-01	25	M342	1 0 1 1 2	

817. C_6H_{10}

3-Hexyne
Diethylacetylene

RN: 928-49-4 **MP** (°C)**:** –103
MW: 82.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	5.586E-01	25	H039	1 2 2 2 1	
6.400E-03	5.257E-01	35	H039	1 2 2 2 1	

818. $C_6H_{10}BrNO_4$

5-Bromo-2-ethyl-5-nitro-1,3-dioxane
2-Ethyl-5-bromo-5-nitro-1,3-dioxane

RN: 54010-85-4 **MP** (°C)**:** 58–59
MW: 240.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.205E-03	7.694E-01	25	L013	1 0 2 1 2	

819. $C_6H_{10}BrNO_4$

5-Bromo-2,2-dimethyl-5-nitro-1,3-dioxane
2,2-Dimethyl-5-bromo-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-2,2-dimethyl-5-nitro-
RN: 60766-57-6 **MP** (°C)**:** 79–81
MW: 240.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.369E-03	1.049E+00	25	L013	1 0 2 1 2	

820. $C_6H_{10}ClN_5$

Deethylatrazine
2-Amino-4-isopropylamino-6-chloro-*s*-triazine
6-Chloro-*N*-(1-methylethyl)-1,3,5-triazine-2,4-diamine
RN: 6190-65-4 **MP** (°C)**:**
MW: 187.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.753E-01	2	B193	1 1 0 0 1	

821. $C_6H_{10}O$

Mesityl oxide
Mesityloxid
RN: 141-79-7 **MP** (°C)**:** –57
MW: 98.15 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.862E-01	2.809E+01	20	D052	1 1 0 0 0	
2.975E-01	2.920E+01	ns	F300	0 0 0 0 2	

822. $C_6H_{10}O$

Cyclohexanone
Cyclohexanon
RN: 108-94-1 **MP** (°C)**:** –47
MW: 98.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-02	1.298E+00	20	D052	1 1 0 0 1	*sic*
2.485E-01	2.439E+01	25	B060	2 0 1 1 1	
8.975E-01	8.809E+01	25	M323	2 2 1 1 2	

823. $C_6H_{10}OS_2$

Allicin
2-Propene-1-sulfinothioic acid *S*-2-propenyl ester
RN: 539-86-6 **MP** (°C)**:** <25
MW: 162.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-01	2.400E+01	10	F300	1 0 0 0 1	

824. $C_6H_{10}O_2$

Methyl vinyl carbinol acetate
1-Methylallyl acetate
3-Buten-2-yl acetate
RN: 6737-11-7 **MP** (°C)**:**
MW: 114.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-01	1.303E+01	26	O012	1 2 1 1 2	
6.953E-02	7.937E+00	50	O012	1 2 1 1 2	
1.718E-01	1.961E+01	75	O012	1 2 1 1 2	

825. $C_6H_{10}O_2$

3-Methyl-1,3-pentadione
1,2-Dimethyl-1,3-butadiene
3,4-Dimethylbutadiene
RN: 4549-74-0 **MP** (°C)**:** –5
MW: 114.15 **BP** (°C)**:** 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.780E-01	1.116E+02	25	M078	2 0 1 0 2	

826. $C_6H_{10}O_2S_4$

Dixanthogen
Ethyl dixanthogen
RN: 502-55-6 **MP** (°C)**:** 28
MW: 242.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.151E-03	22	P076	1 2 1 1 1	
1.140E-05	2.763E-03	25	H102	1 2 1 2 2	
<2.06E-06	<5.00E-04	25	M161	1 0 0 0 0	
1.250E-05	3.030E-03	ns	L083	0 0 0 0 0	EFG, pH 3–9

827. $C_6H_{10}O_3$
Ethyl acetoacetate
Acetessigsaeure-aethyl ester
Acetoacetic acid ethyl ester
RN: 141-97-9 **MP** (°C)**:** –45
MW: 130.14 **BP** (°C)**:** 180.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.613E-01	1.251E+02	10.5	D041	1 0 0 0 2	
8.529E-01	1.110E+02	16.50	F300	1 0 0 0 2	

828. $C_6H_{10}O_4$
2,2-Dimethylsuccinic acid
α,α-Dimethylbernsteinsaeure
RN: 597-43-3 **MP** (°C)**:** 140.5
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.790E-01	7.000E+01	14	F300	1 0 0 0 2	

829. $C_6H_{10}O_4$
sym-Dimethylsuccinic acid
Acide Dimethylsuccinique-*sym*
RN: 608-40-2 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	3.000E+02	15	M051	1 0 0 0 2	

830. $C_6H_{10}O_4$
n-Propylmalonic acid
Acide *n*-propylmalonique
RN: 616-62-6 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E+00	4.560E+02	0	M051	1 0 0 0 2	
4.112E+00	6.010E+02	15	M051	1 0 0 0 2	
4.790E+00	7.000E+02	25	M051	1 0 0 0 2	
6.459E+00	9.440E+02	50	M051	1 0 0 0 2	

831. $C_6H_{10}O_4$
Ethylene glycol diacetate
Glycol diacetate
RN: 111-55-7 **MP** (°C)**:** –31
MW: 146.14 **BP** (°C)**:** 190

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.756E+02	20	D052	1 1 0 0 2	
9.661E-01	1.412E+02	20	M062	1 0 0 0 2	
8.526E-01	1.246E+02	22	F300	1 0 0 0 2	
1.034E+00	1.511E+02	24.50	O005	2 0 2 2 2	
1.070E+00	1.564E+02	25	F064	1 0 0 0 2	
1.220E-01	1.783E+01	ns	F014	0 0 0 0 2	

832. $C_6H_{10}O_4$
DL-2,3-Dimethylsuccinic acid
DL-α,α′-Dimethylbernsteinsaeure
RN: 13545-04-5 **MP** (°C)**:** 120
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-01	3.000E+01	14	F300	1 0 0 0 0	

833. $C_6H_{10}O_4$
Adipic acid
Adipinsaeure
RN: 124-04-9 **MP** (°C)**:** 152
MW: 146.14 **BP** (°C)**:** 337.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.431E-02	7.937E+00	0	M043	1 0 0 0 0	
6.766E-02	9.888E+00	4.99	A339	0 0 0 0 0	
6.775E-02	9.901E+00	10	M043	1 0 0 0 1	
7.853E-02	1.148E+01	9.99	A339	0 0 0 0 0	
1.061E-01	1.551E+01	14.99	A339	0 0 0 0 0	
9.580E-02	1.400E+01	15	F300	1 0 0 0 1	
9.580E-02	1.400E+01	15	L041	1 0 0 1 1	
9.580E-02	1.400E+01	15	M051	1 0 0 0 1	
1.303E-01	1.904E+01	19.99	A339	0 0 0 0 0	
1.011E-01	1.478E+01	20	D041	1 0 0 0 1	
1.276E-01	1.865E+01	20	M043	1 0 0 0 1	
9.856E-02	1.440E+01	20	M171	1 0 0 0 1	
9.000E-02	1.315E+01	20	S006	1 0 0 0 1	
4.824E-01	7.050E+01	21	B040	1 0 1 1 2	*sic*
1.664E-01	2.432E+01	24.99	A339	0 0 0 0 0	
2.216E-03	3.239E-01	25	K035	2 0 0 0 2	*sic*
2.053E-01	3.001E+01	29.99	A339	0 0 0 0 0	

(*continued*)

833. $C_6H_{10}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-01	2.913E+01	30	M043	1 0 0 0 1	
2.045E-01	2.988E+01	34.10	A031	1 2 2 2 2	
2.546E-01	3.721E+01	34.99	A339	0 0 0 0 0	
2.933E-01	4.287E+01	39.3	G302	2 2 2 2 0	EFG
3.274E-01	4.785E+01	39.99	A339	0 0 0 0 0	
3.333E-01	4.871E+01	40	A031	1 2 2 2 2	
3.382E-01	4.943E+01	40	B088	1 0 0 0 1	
3.258E-01	4.762E+01	40	M043	1 0 0 0 1	
4.383E-01	6.406E+01	44.99	A339	0 0 0 0 0	
5.516E-01	8.062E+01	49.99	A339	0 0 0 0 0	
5.788E-01	8.458E+01	50	A031	1 2 2 2 2	
7.508E-01	1.097E+02	54.99	A339	0 0 0 0 0	
1.011E+00	1.477E+02	59.99	A339	0 0 0 0 0	
1.024E+00	1.497E+02	60	A031	1 2 2 2 2	
1.044E+00	1.525E+02	60	M043	1 0 0 0 1	
1.130E+00	1.652E+02	64.99	A339	0 0 0 0 0	
1.740E+00	2.543E+02	70	A031	1 2 2 2 2	
2.818E+00	4.118E+02	80	M043	1 0 0 0 1	
3.330E+00	4.867E+02	87.10	A031	1 2 2 2 2	
4.277E+00	6.250E+02	100	F300	1 0 0 0 2	
4.211E+00	6.154E+02	100	M043	1 0 0 0 2	
1.662E-01	2.430E+01	rt	H431	0 0 0 0 0	

834. $C_6H_{10}O_4$

Methyl α-acetoxypropionate
Methyl 2-acetoxypropionate
Methyl *O*-acetyllactate
Methyl 2-acetyloxypropanoate

RN: 6284-75-9 **MP** (°C)**:**
MW: 146.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-01	8.120E+01	25	R006	2 2 0 1 2	

835. $C_6H_{10}O_5$

Propanoic acid, 2-[(methoxycarbonyl)oxy]-, methyl ester
Carbonic acid, methyl ester, ester with methyl lactate

RN: 6288-11-5 **MP** (°C)**:**
MW: 162.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-01	3.911E+01	25	R007	0 0 0 0 0	

836. $C_6H_{10}O_8$
D-Talogalactaric acid
D-Taloschleimsaeure
D-Galactaric acid
Galactaric acid
Schleimsaeure
RN: 526-99-8 **MP** (°C)**:** > 230
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	3.289E+00	14	D041	1 0 0 0 1	
1.570E-02	3.300E+00	14	F300	1 0 0 0 1	
8.090E-02	1.700E+01	100	F300	1 0 0 0 1	

837. $C_6H_{11}Br$
Bromocyclohexane
Cyclohexyl bromide
RN: 108-85-0 **MP** (°C)**:**
MW: 163.06 **BP** (°C)**:** 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.012E-03	8.173E-01	ns	S460	0 0 0 0 0	

838. $C_6H_{11}BrN_2O_2$
α-Methyl-γ-bromo-butanoic ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.658E-02	1.039E+01	ns	F056	0 2 2 2 1	

839. $C_6H_{11}BrN_2O_2$
α-Bromo-isovaleric ureide
Butanamide, *N*-(aminocarbonyl)-2-bromo-3-methyl-
Dormigene
Pivadorn
Pivadorm
Isobromyl
RN: 496-67-3 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.531E-02	1.903E+01	ns	F057	0 2 2 2 2	

840. $C_6H_{11}BrN_2O_2$
3-Bromo-2-methyl-butanoic ureide
Urea, (2-bromo-2-methylbutyryl)-
DL-*N*-(2-Bromo-2-methylbutanoyl)urea
RN: 14368-76-4 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	3.101E+01	ns	F056	0 2 2 2 1	

841. $C_6H_{11}BrN_2O_2$
β-Bromo-valeric acid ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.470E-02	7.740E+00	ns	F056	0 2 2 2 1	

842. $C_6H_{11}BrN_2O_2$
γ-Bromo-valeric acid ureide
RN: **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.307E-02	9.607E+00	ns	F056	0 2 2 2 1	

843. $C_6H_{11}BrN_2O_2$
α-Bromo-valeric acid ureide
Pentanamide, *N*-(aminocarbonyl)-2-bromo-
RN: 66947-87-3 **MP** (°C)**:**
MW: 223.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-02	8.232E+00	ns	F056	0 2 2 2 1	
3.703E-02	8.261E+00	ns	F057	0 2 2 2 2	

844. $C_6H_{11}NO$
Caprolactam
ε-Caprolactam
RN: 105-60-2 **MP** (°C)**:** 70
MW: 113.16 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.776E+00	4.273E+02	5.70	B201	2 2 2 1 2	
3.850E+00	4.357E+02	10.30	B201	2 2 2 1 2	

845. $C_6H_{11}NO$

Cyclohexanone oxime
Antioxidant D
(Hydroxyimino)cyclohexane

RN: 100-64-1 **MP** (°C)**:** 90
MW: 113.16 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.409E-01	1.594E+01	25.5	K087	1 0 0 0 2	
1.580E-01	1.787E+01	32.0	K087	1 0 0 0 2	
1.648E-01	1.865E+01	36.8	K087	1 0 0 0 2	
1.936E-01	2.191E+01	44.0	K087	1 0 0 0 2	
2.155E-01	2.439E+01	48.8	K087	1 0 0 0 2	
2.715E-01	3.073E+01	60.4	K087	1 0 0 0 2	
2.922E-01	3.307E+01	63.7	K087	1 0 0 0 2	
3.194E-01	3.614E+01	76.2	K087	1 0 0 0 2	
3.456E-01	3.911E+01	83.1	K087	1 0 0 0 2	
4.039E-01	4.571E+01	95.2	K087	1 0 0 0 2	
4.939E-01	5.589E+01	110.7	K087	1 0 0 0 2	
5.743E-01	6.498E+01	120	K087	1 0 0 0 2	
7.386E-01	8.358E+01	131	K087	1 0 0 0 2	

846. $C_6H_{11}NO_2S$

2,2-Dimethylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2,2-dimethyl-
Thiazolidine-4-carboxylic acid, 2,2-dimethyl-

RN: 42607-20-5 **MP** (°C)**:**
MW: 161.22 **BP** (°C)**:** 317.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	4.837E+01	21	B414	1 0 0 1 1	very fast and extent decompostion, uncertain value

847. $C_6H_{11}NO_4$

α-Aminoadipic acid
2-Aminohexanedioic acid
α-Amino-adipinsaeure

RN: 542-32-5 **MP** (°C)**:**
MW: 161.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.365E-02	2.200E+00	20	F300	1 0 0 0 1	

848. $C_6H_{11}NO_4$
Glycine, *N*-(carboxymethyl)-, 1-ethyl ester
AcGlyOEt
Acetic acid, iminodi-, monoethyl ester
RN: 21885-31-4 **MP** (°C)**:**
MW: 161.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.074E-03	1.140E+00	27	D036	0 0 0 0 0	

849. $C_6H_{11}N_2O_4PS_3$
Methidathion
Supracide
S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl) *O,O*-dimethyl phosphorodithioate
Ultracide
Somanil
S-2,3-Dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl *O,O*-dimethylphosphorodithioate
RN: 950-37-8 **MP** (°C)**:**
MW: 302.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.186E-04	1.870E-01	20	B300	2 2 1 1 2	
8.269E-04	2.500E-01	20	F311	1 2 2 2 1	
7.938E-04	2.400E-01	25	M161	1 0 0 0 2	

850. $C_6H_{11}N_3O_6$
Glycine tripeptide
RN: **MP** (°C)**:**
MW: 221.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.127E-01	4.705E+01	20	B032	1 2 2 1 2	
2.907E-01	6.430E+01	25	B032	1 2 2 1 2	
3.565E-01	7.884E+01	29.80	B032	1 2 2 1 2	

851. C_6H_{12}
Methylcyclopentane
MCP
RN: 96-37-7 **MP** (°C)**:** –142
MW: 84.16 **BP** (°C)**:** 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	K119	1 0 0 0 2	
4.990E-04	4.200E-02	25	M001	2 1 2 2 2	
5.062E-04	4.260E-02	25	M002	2 1 2 2 2	

(*continued*)

851. C_6H_{12} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	P051	2 1 1 2 2	
4.967E-04	4.180E-02	25.00	P007	2 1 2 2 2	
4.990E-04	4.200E-02	ns	H123	0 0 0 0 0	

852. C_6H_{12}

Cyclohexane
Cyclohexan

RN: 110-82-7 **MP** (°C)**:** 7
MW: 84.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.734E-04	8.192E-02	4.8	L007	2 1 1 2 2	
9.734E-04	8.192E-02	5.1	L007	2 0 1 1 2	
1.054E-03	8.869E-02	14.8	L007	2 1 1 2 2	
1.054E-03	8.869E-02	15.2	L007	2 0 1 1 2	
9.505E-04	8.000E-02	16	D047	1 0 0 1 1	
<5.94E-04	<5.00E-02	17	F300	1 0 0 0 0	
4.396E-04	3.700E-02	20	M337	2 1 2 2 2	
6.178E-04	5.200E-02	23.5	S171	2 1 2 2 2	
1.055E-03	8.883E-02	24.8	L007	2 1 1 2 2	
9.505E-04	7.999E-02	25	G068	1 0 1 0 0	
6.939E-04	5.840E-02	25	G313	2 1 1 2 2	
1.426E-03	1.200E-01	25	K112	1 0 2 1 1	
7.901E-04	6.650E-02	25	K119	1 0 0 0 2	
6.737E-04	5.670E-02	25	L002	2 2 2 2 2	
6.535E-04	5.500E-02	25	M001	2 1 2 2 2	
6.535E-04	5.500E-02	25	M002	2 1 2 2 2	
6.535E-04	5.500E-02	25	M040	1 0 0 1 1	
6.832E-04	5.750E-02	25	M132	2 2 2 1 2	
7.901E-04	6.650E-02	25	P051	2 1 1 2 2	
6.270E-04	5.277E-02	25	S359	2 1 2 2 2	
7.901E-04	6.650E-02	25.00	P007	2 1 2 2 2	
1.055E-03	8.883E-02	34.8	L007	2 1 1 2 2	
1.055E-03	8.883E-02	35.2	L007	2 0 1 1 2	
5.389E-04	4.535E-02	38	K055	1 2 0 1 1	
1.085E-03	9.131E-02	44.8	L007	2 1 1 2 2	
1.085E-03	9.131E-02	45.2	L007	2 0 1 1 2	
1.426E-03	1.200E-01	50	L097	1 1 1 1 1	
2.020E-03	1.700E-01	56	G068	1 0 1 0 1	
3.222E-04	2.712E-02	71	K055	1 2 0 1 1	
3.326E-03	2.799E-01	94	G068	1 0 1 0 1	
1.200E-04	1.010E-02	ns	D348	0 0 0 0 0	
6.535E-04	5.500E-02	ns	H123	0 0 0 0 0	
5.000E-03	4.208E-01	ns	H333	0 1 0 1 0	EFG
9.505E-04	8.000E-02	ns	M010	0 0 0 0 0	
6.642E-04	5.590E-02	ns	M175	0 0 2 1 2	

853. C_6H_{12}
4-Methyl-1-pentene
4-Methylpentene
Isohexene
RN: 691-37-2 **MP** (°C)**:** –154
MW: 84.16 **BP** (°C)**:** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.703E-04	4.800E-02	25	M001	2 1 2 2 1	

854. C_6H_{12}
2-Methyl-1-pentene
4-Methyl-4-pentene
RN: 763-29-1 **MP** (°C)**:** –136
MW: 84.16 **BP** (°C)**:** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.268E-04	7.800E-02	25	M001	2 1 2 2 2	

855. C_6H_{12}
1-Hexene
1-*n*-Hexene
Hexene
Dialen 6
RN: 592-41-6 **MP** (°C)**:** –140
MW: 84.16 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.822E-04	4.900E-02	23	C332	0 0 0 0 0	
6.583E-04	5.540E-02	25	L002	2 2 2 2 2	
5.941E-04	5.000E-02	25	M001	2 1 2 2 2	
5.941E-04	5.000E-02	25	M040	1 0 0 1 1	
8.280E-04	6.969E-02	25	M342	1 0 1 1 2	

856. $C_6H_{12}ClNO$
Acetamide, 2-chloro-*N*,*N*-diethyl-
CDEA
RN: 2315-36-8 **MP** (°C)**:**
MW: 149.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.264E-01	7.877E+01	25	B185	0 0 0 0 0	

857. $C_6H_{12}Cl_2O$
Dichloroisopropyl ether
bis(2-Chloro-1-methylethyl) ether
DCIP
β,β′-Dichlorodiisopropyl ether
2,2′-Oxybis[1-chloropropane]
Pichloram
RN: 63283-80-7 **MP** (°C)**:**
MW: 171.07 **BP** (°C)**:** 187.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.921E-03	1.697E+00	20	M062	1 0 0 0 1	

858. $C_6H_{12}Cl_2O_2$
1,2-bis(2-Chloroethoxy)ethane
Triglycol dichloride
RN: 112-26-5 **MP** (°C)**:** 121
MW: 187.07 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.916E-02	1.855E+01	20	M062	1 0 0 0 2	

859. $C_6H_{12}Cl_3O_4P$
tris-(2-Chloroethyl) phosphate
Tri-β-chloroethyl phosphate
RN: 115-96-8 **MP** (°C)**:**
MW: 285.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.01E-04	<2.00E-01	25	B070	1 2 0 1 0	

860. $C_6H_{12}NO_3PS_2$
Diethyl 1,3-dithietan-2-ylidenephosphoramidate
Nematak
AC 64475
Geofos
Fosthietan
CL 64475
RN: 21548-32-3 **MP** (°C)**:**
MW: 241.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.072E-01	5.000E+01	25	M161	1 0 0 0 1	

861. $C_6H_{12}NO_4PS_2$
Formothion
O,*O*-Dimethyl *S*-(*N*-methyl-*N*-formylcarbamoylmethyl) dithiophosphate
RN: 2540-82-1 **MP** (°C)**:**
MW: 257.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-02	2.600E+00	24	M161	1 0 0 0 1	

862. $C_6H_{12}N_2O$
N-Nitrosohexamethyleneimine
NHMI
RN: 932-83-2 **MP** (°C)**:**
MW: 128.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.282E+01	24	M031	1 1 1 1 1	

863. $C_6H_{12}N_2O_2$
2,6-Dimethylnitrosomorpholine
DMNM
RN: 1456-28-6 **MP** (°C)**:**
MW: 144.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-01	1.240E+02	24	M031	1 1 1 1 1	

864. $C_6H_{12}N_2O_2$
Adipamide
Adipinsaeurediamid
RN: 628-94-4 **MP** (°C)**:**
MW: 144.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.052E-02	4.400E+00	12.20	F300	1 0 0 0 1	

865. $C_6H_{12}N_2O_3$
Daminozide
N-Dimethylamino-β-carbamyl propionic acid
Succinic acid 2,2-dimethylhydrazide
Alar
DMASA
RN: 1596-84-5 **MP** (°C)**:** 155
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-01	1.000E+02	25	M161	1 0 0 0 2	

866. $C_6H_{12}N_2O_3$
δ-Aminovaleric hydantoic acid
δ-Uramidovaleric acid
RN: **MP** (°C)**:** 179
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.740E-02	2.787E+00	25	M024	1 2 0 1 2	

867. $C_6H_{12}N_2O_3S$
Methomyl
Acetamidic acid
N-[(methyl-carbamoyl)oxy]-, methyl ester
Carbamic acid
Lannabait
Nudrin
RN: 16752-77-5 **MP** (°C)**:** 78
MW: 192.24 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.548E-01	6.821E+01	ns	R424	0 0 0 0 0	

868. $C_6H_{12}N_2O_4S_2$
L-Cystine
3,3′-Dithiobis(2-aminopropanoic acid)
RN: 56-89-3 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.021E-03	4.858E-01	20	H082	1 2 1 1 2	isomeric
7.905E-04	1.900E-01	20	H082	1 2 1 1 2	plate cystine
6.910E-04	1.660E-01	24.99	C404	2 1 2 2 1	
7.000E-02	1.682E+01	25	C405	2 1 2 2 2	intrinsic zwit

(*continued*)

868. $C_6H_{12}N_2O_4S_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-04	1.090E-01	25	D017	1 0 0 0 2	
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.661E-04	1.120E-01	25	L001	1 0 1 1 2	pH 6.0
4.910E-04	1.180E-01	27	D036	0 0 0 0 0	
7.100E-04	1.706E-01	34.99	C404	2 1 2 2 1	
8.500E-04	2.043E-01	44.99	C404	2 1 2 2 1	
2.163E-03	5.197E-01	75	D041	1 0 0 0 1	
4.536E-04	1.090E-01	rt	B103	0 0 0 0 2	

869. $C_6H_{12}N_2O_4S$

DL-Lanthionine

L-Cysteine, *S*-[(2*R*)-2-amino-2-carboxyethyl]-

RN: 922-55-4 **MP** (°C)**:** 280

MW: 208.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.193E-03	1.498E+00	25	D041	1 0 0 0 1	

870. $C_6H_{12}N_2O_4S_2$

Mesocystine

meso-Cystine

RN: 6020-39-9 **MP** (°C)**:**

MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	5.600E-02	25	L001	1 0 1 1 1	pH 6.0

871. $C_6H_{12}N_2O_4S_2$

D-Cystine

D-(+)-3,3′-Dithiobis(2-aminopropanoic acid)

RN: 349-46-2 **MP** (°C)**:** 227

MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.702E-04	1.130E-01	25	L001	1 0 1 1 2	pH 6.0

872. $C_6H_{12}N_2O_4S_2$
DL-Cystine
Cystine
RN: 923-32-0 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-04	4.900E-02	25	D041	1 0 0 0 1	
2.372E-04	5.700E-02	25	L001	1 0 1 1 1	pH 6.0

873. $C_6H_{12}N_2S_4$
Thiram
Tetramethylthioperoxydicarbonothioic diamine
Tetramethylthiuram disulfide
N,*N*′-(Dithiodicarbonothioyl)bis(*N*-methylmethanamine)
Arasan
Nomersan
RN: 137-26-8 **MP** (°C)**:** 155.5
MW: 240.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.413E-05	1.782E-02	ns	R427	0 0 0 0 0	
1.248E-04	3.000E-02	rt	M161	0 0 0 0 1	

874. $C_6H_{12}N_2S_4Zn$
Ziram
Zinc *bis* dimethyldithiocarbamate
Corozate
Karbam white
Fuklasin
Fuclasin
RN: 137-30-4 **MP** (°C)**:** 240
MW: 305.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-04	6.500E-02	20	F300	1 0 0 0 1	
1.308E-05	4.000E-03	20	F311	1 2 2 2 1	*sic*
2.125E-04	6.500E-02	25	M161	1 0 0 0 1	

875. $C_6H_{12}N_4$
Methenamine
Hexamethylen-tetramin
RN: 100-97-0 **MP** (°C)**:**
MW: 140.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.231E+00	3.128E+02	1.99	B442	0 0 0 0 0	
2.202E+00	3.087E+02	3.99	B442	0 0 0 0 0	
2.183E+00	3.060E+02	5.99	B442	0 0 0 0 0	
2.149E+00	3.012E+02	9.99	B442	0 0 0 0 0	
2.254E+00	3.161E+02	10.99	B442	0 0 0 0 0	
2.250E+00	3.154E+02	11.99	B442	0 0 0 0 0	
3.200E+00	4.486E+02	12	F300	1 0 0 0 2	
2.234E+00	3.131E+02	14.99	B442	0 0 0 0 0	
2.191E+00	3.072E+02	19.99	B442	0 0 0 0 0	
2.156E+00	3.023E+02	24.99	B442	0 0 0 0 0	
2.193E+00	3.074E+02	29.99	B442	0 0 0 0 0	
2.218E+00	3.110E+02	34.99	B442	0 0 0 0 0	
2.233E+00	3.131E+02	39.99	B442	0 0 0 0 0	

876. $C_6H_{12}N_4O_2$
2,6-Dimethyldinitrosopiperazine
DMDNP
RN: 55380-34-2 **MP** (°C)**:**
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.066E+01	24	M031	1 1 1 1 1	

877. $C_6H_{12}N_5O_2PS_2$
Menazon
O,*O*-Dimethyl *S*-(4,6-diamino-1,3,5-triazinyl-2-methyl) dithiophosphate
RN: 78-57-9 **MP** (°C)**:**
MW: 281.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.532E-04	2.400E-01	20	M161	1 0 0 0 1	
3.551E-03	9.990E-01	ns	M061	0 0 0 0 0	

878. $C_6H_{12}O$
Pinacolone
3,3-Dimethyl-2-butanone
3,3-Dimethylbutanone-2
RN: 75-97-8 **MP** (°C)**:** –52.5
MW: 100.16 **BP** (°C)**:** 106.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.376E-01	2.380E+01	15	F300	1 0 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	
1.862E-01	1.865E+01	25	G030	1 2 0 0 2	
1.817E-01	1.820E+01	25	K072	1 0 1 1 1	
1.736E-01	1.739E+01	30	G030	1 2 0 0 2	

879. $C_6H_{12}O$
Cyclohexanol
1-Cyclohexanol
Naxol
Cyclohexyl alcoho
Adrona
Hydrophenol
RN: 108-93-0 **MP** (°C)**:** 23
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.357E-01	5.366E+01	11	F052	1 1 1 0 2	
5.391E-01	5.400E+01	11	F300	1 0 0 0 1	
1.296E-02	1.298E+00	20	D052	1 1 0 0 1	*sic*
3.283E-01	3.288E+01	25	B019	1 0 1 2 0	
3.283E-01	3.288E+01	25	B092	2 1 1 1 2	
3.469E-01	3.475E+01	25	C108	2 2 2 2 2	
3.800E-01	3.806E+01	25	F044	1 0 0 0 1	
3.766E-01	3.772E+01	25	H028	2 0 2 0 2	
3.655E-01	3.661E+01	35	C108	2 2 2 2 2	
3.264E-01	3.269E+01	60	B092	2 1 1 1 2	
3.766E-01	3.772E+01	ns	A406	0 0 0 0 1	

880. $C_6H_{12}O$
Isopropylacetone
4-Methyl-2-pentanone
Methyl isobutyl ketone
RN: 108-10-1 **MP** (°C)**:** –80
MW: 100.16 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.070E-01	3.075E+01	0	G032	1 2 1 1 2	
2.310E-01	2.314E+01	10	G032	1 2 1 1 2	
1.871E-01	1.874E+01	20	D052	1 1 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	

(*continued*)

880. $C_6H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-01	1.961E+01	22.00	O005	2 0 2 2 0	
1.862E-01	1.865E+01	24.6	H121	2 0 0 0 1	
1.862E-01	1.865E+01	25	B060	2 0 1 1 1	
1.717E-01	1.720E+01	25	C329	1 1 1 1 1	average
1.871E-01	1.874E+01	25	G030	1 2 0 0 2	
2.340E-01	2.344E+01	25	K103	1 2 2 2 1	
1.862E-01	1.865E+01	25	L082	1 1 2 1 1	
1.736E-01	1.739E+01	25	L319	1 0 2 1 2	
1.817E-01	1.820E+01	25	M087	1 1 2 1 2	
1.669E-01	1.672E+01	25	R320	1 0 1 1 1	
1.746E-01	1.749E+01	30	G030	1 2 0 0 2	
1.660E-01	1.663E+01	30	G032	1 2 1 1 2	
1.410E-01	1.412E+01	50	G032	1 2 1 1 2	
4.720E+01	4.728E+03	53.0	R308	2 2 1 1 2	
1.669E-01	1.672E+01	70	L082	1 1 2 1 1	
1.370E-01	1.372E+01	75	G032	1 2 1 1 2	
4.300E+01	4.307E+03	97.0	R308	2 2 1 1 2	
4.088E+01	4.094E+03	108.0	R308	2 2 1 1 2	
3.902E+01	3.909E+03	120.0	R308	2 2 1 1 2	
3.333E-01	3.339E+01	125.0	R308	2 2 1 1 1	
5.278E-01	5.286E+01	151.0	R308	2 2 1 1 1	
3.425E+01	3.431E+03	153.0	R308	2 2 1 2 2	

881. $C_6H_{12}O$

2-Ethylbutanal
Ethyl butyraldehyde
2-Ethylbutyraldehyde
Diethyl acetaldehyde; ethyl butyraldehyde
Diethyl acetaldehyde
Ethyl butyraldehyde

RN: 97-96-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	3.025E+00	ns	S460	0 0 0 0 0	

882. $C_6H_{12}O$

Caproic aldehyde
Hexaldehyde
n-Hexanal

RN: 66-25-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-01	5.590E+01	0	C423	0 0 0 0 0	
4.493E-01	4.500E+01	4	C423	0 0 0 0 0	

(*continued*)

882. $C_6H_{12}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.155E-01	3.160E+01	10	C423	0 0 0 0 0	
4.992E-02	5.000E+00	25	A049	1 0 1 0 1	
1.907E-01	1.910E+01	25	C435	0 0 0 0 0	
4.792E-02	4.800E+00	25	J418	0 0 0 0 0	

883. $C_6H_{12}O$

4-Methyl-3-pentanone
4-Methylpentanone-3
RN: 565-69-5 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.601E-01	1.604E+01	20	G030	1 2 0 0 2	
1.495E-01	1.497E+01	25	G030	1 2 0 0 2	
1.398E-01	1.400E+01	30	G030	1 2 0 0 2	
1.549E-01	1.551E+01	ns	S460	0 0 0 0 0	

884. $C_6H_{12}O$

3-Methyl-2-pentanone
3-Methylpentanone-2
RN: 565-61-7 **MP** (°C)**:** <25
MW: 100.16 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-01	2.210E+01	20	G030	1 2 0 0 2	
2.044E-01	2.047E+01	25	G030	1 2 0 0 2	
1.890E-01	1.893E+01	30	G030	1 2 0 0 2	

885. $C_6H_{12}O$

3-Hexanone
Hexanone-3
RN: 589-38-8 **MP** (°C)**:** –55.5
MW: 100.16 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-01	1.546E+01	20	G030	1 2 0 0 2	
1.446E-01	1.449E+01	25	G030	1 2 0 0 2	
1.359E-01	1.361E+01	30	G030	1 2 0 0 2	

886. $C_6H_{12}O$
2-Methyl-4-penten-3-ol
2-Methylpenten-4-ol-3
RN: 4798-45-2 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-01	3.185E+01	20	G031	1 0 0 0 2	
2.964E-01	2.969E+01	25	G031	1 0 0 0 2	
2.804E-01	2.809E+01	30	G031	1 0 0 0 2	

887. $C_6H_{12}O$
1-Hexen-3-ol
Hexen-1-ol-3
RN: 4798-44-1 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E-01	2.648E+01	20	G031	1 0 0 0 2	
2.454E-01	2.458E+01	25	G031	1 0 0 0 2	
2.302E-01	2.306E+01	30	G031	1 0 0 0 2	

888. $C_6H_{12}O$
Methyl butyl ketone
2-Hexanone
Methyl *n*-butyl ketone
RN: 591-78-6 **MP** (°C)**:** –57
MW: 100.16 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-01	4.330E+01	0	C423	0 0 0 0 0	
3.335E-01	3.340E+01	4	C423	0 0 0 0 0	
2.386E-01	2.390E+01	10	C423	0 0 0 0 0	
2.040E-01	2.043E+01	10	G032	1 2 1 1 2	
2.192E-02	2.195E+00	20	D052	1 1 0 0 1	*sic*
1.717E-01	1.720E+01	20	G030	1 2 0 0 2	
1.617E-01	1.620E+01	25	C435	0 0 0 0 0	
1.611E-01	1.614E+01	25	G030	1 2 0 0 2	
1.997E-01	2.000E+01	25	J418	0 0 0 0 0	
3.320E-01	3.326E+01	25	P055	1 0 0 0 2	
1.505E-01	1.507E+01	30	G030	1 2 0 0 2	
1.450E-01	1.452E+01	30	G032	1 2 1 1 2	
1.475E-01	1.478E+01	38	J020	2 1 2 1 1	
1.240E-01	1.242E+01	50	G032	1 2 1 1 2	

889. $C_6H_{12}O$
4-Hexen-3-ol
Hexen-4-ol-3
RN: 4798-58-7 **MP** (°C)**:**
MW: 100.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-01	3.902E+01	20	G031	1 0 0 0 2	
3.664E-01	3.670E+01	25	G031	1 0 0 0 2	
3.451E-01	3.456E+01	30	G031	1 0 0 0 2	

890. $C_6H_{12}O_2$
3-Hydroxy-2,2-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2,2-dimethyl-
2,2-Dimethyltetrahydrofuran-3-ol
RN: 101398-19-0 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.826E-01	9.091E+01	rt	B066	0 2 0 0 1	

891. $C_6H_{12}O_2$
Diethylacetic acid
2-Ethylbutyric acid
2-Ethyl-butanoic acid
Ethylbutyric acid
RN: 88-09-5 **MP** (°C)**:** –15
MW: 116.16 **BP** (°C)**:** 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.147E-02	2.494E+00	25	O011	1 0 1 1 1	

892. $C_6H_{12}O_2$
n-Caproic acid
n-Capronsaeure
RN: 142-62-1 **MP** (°C)**:** –3.4
MW: 116.16 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.438E-02	8.640E+00	0	B136	1 0 2 1 2	
7.610E-02	8.840E+00	15	F300	1 0 0 0 2	
8.333E-02	9.680E+00	20	B136	1 0 2 1 2	
8.270E-02	9.607E+00	20	D041	1 0 0 0 1	
8.253E-02	9.587E+00	20	R001	1 1 1 1 2	
8.675E-02	1.008E+01	25	H028	2 0 2 0 2	

(*continued*)

892. $C_6H_{12}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.760E-02	1.018E+01	25	H122	1 0 0 0 2	
8.608E-02	9.999E+00	25	H339	2 2 1 2 2	
9.367E-02	1.088E+01	25	O011	1 0 1 1 1	
8.772E-02	1.019E+01	30	B136	1 0 2 1 2	
8.684E-02	1.009E+01	30	R001	1 1 1 1 2	
9.282E-02	1.078E+01	35	H339	2 2 1 2 2	
9.427E-02	1.095E+01	45	B136	1 0 2 1 2	
9.324E-02	1.083E+01	45	R001	1 1 1 1 2	
1.008E-01	1.171E+01	60	B136	1 0 2 1 2	
9.956E-02	1.156E+01	60	D041	1 0 0 0 2	
9.964E-02	1.157E+01	60	R001	1 1 1 1 2	
7.374E-02	8.566E+00	.0	R001	1 1 1 1 2	
8.692E-02	1.010E+01	ns	A406	0 0 0 0 1	

893. $C_6H_{12}O_2$

n-Butyl acetate
Essigsaeure-n-butyl ester
n-Butylacetat
Butyl acetate
1-Butyl acetate

RN: 123-86-4 **MP** (°C)**:** –90
MW: 116.16 **BP** (°C)**:** 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-02	4.282E+00	20	D052	1 1 0 0 0	
8.609E-02	1.000E+01	22	F300	1 0 0 0 0	
5.814E-02	6.754E+00	25	B060	2 0 1 1 1	
7.171E-02	8.330E+00	25	L319	1 0 2 1 2	
1.935E-01	2.248E+01	25	P055	1 0 0 0 1	
2.489E-02	2.892E+00	30	N330	2 2 2 1 2	
7.679E-02	8.920E+00	30	R318	1 1 0 1 0	
5.020E-02	5.831E+00	37	E028	1 0 1 1 2	
5.899E-02	6.853E+00	50	O012	1 2 1 1 2	

894. $C_6H_{12}O_2$

Pentyl formate
n-Amyl formate

RN: 638-49-3 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	2.904E+00	22	S006	1 0 0 0 1	

895. $C_6H_{12}O_2$
Ethyl butyrate
Butanoic acid ethyl ester
Ethyl butanoate
Butyric ether
RN: 105-54-4 **MP** (°C)**:** –135.4
MW: 116.16 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-02	2.800E+00	0	C423	0 0 0 0 0	
2.763E-02	3.210E+00	4	C423	0 0 0 0 0	
3.151E-02	3.660E+00	10	C423	0 0 0 0 0	
4.198E-02	4.876E+00	20	D052	1 1 0 0 1	
5.310E-02	6.168E+00	22	F001	1 0 1 2 2	
4.300E-02	4.995E+00	22	S006	1 0 0 0 1	
3.702E-02	4.300E+00	25	C435	0 0 0 0 0	
6.832E-02	7.937E+00	30	R318	1 1 0 1 0	

896. $C_6H_{12}O_2$
sec-Butyl acetate
DL-*sec*-Butyl acetate
RN: 105-46-4 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.305E-02	6.162E+00	20	D052	1 1 0 0 0	

897. $C_6H_{12}O_2$
3-Hydroxy-2,5-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2,5-dimethyl-
RN: 30003-26-0 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.435E+00	1.667E+02	rt	B066	0 2 0 0 1	

898. $C_6H_{12}O_2$
Propyl propionate
Propionic acid *N*-propyl ester
n-Propyl propionate
RN: 106-36-5 **MP** (°C)**:**
MW: 116.16 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.808E+00	22	S006	1 0 0 0 0	

899. $C_6H_{12}O_2$
Isobutyl acetate
Acetic acid isobutyl ester
Essigsaeureisobutyl ester
RN: 110-19-0 **MP** (°C)**:** –99
MW: 116.16 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.502E-02	7.553E+00	14.60	L310	2 2 1 1 2	
5.729E-02	6.655E+00	20	D052	1 1 0 0 1	
5.800E-02	6.737E+00	20	F001	1 0 1 2 1	
5.768E-02	6.700E+00	20	F300	1 0 0 0 1	
6.154E-02	7.149E+00	24.90	L310	2 2 1 1 2	
5.390E-02	6.261E+00	25	B060	2 0 1 1 1	
5.967E-02	6.932E+00	47.90	L310	2 2 1 1 2	
6.154E-02	7.149E+00	67.60	L310	2 2 1 1 2	
6.493E-02	7.543E+00	74.90	L310	2 2 1 1 2	
6.502E-02	7.553E+00	75.20	L310	2 2 1 1 2	
6.875E-02	7.986E+00	84.80	L310	2 2 1 1 2	
7.205E-02	8.369E+00	93.20	L310	2 2 1 1 2	
8.253E-02	9.587E+00	111.50	L310	2 2 1 1 2	
8.540E-02	9.921E+00	115.70	L310	2 2 1 1 2	
1.026E-01	1.192E+01	147.10	L310	2 2 1 1 2	

900. $C_6H_{12}O_3$
Paraldehyde
Paraldehyd
RN: 123-63-7 **MP** (°C)**:** 12.6
MW: 132.16 **BP** (°C)**:** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.853E-01	1.170E+02	8.5	P059	1 1 1 0 1	
8.377E-01	1.107E+02	11.5	P059	1 1 1 0 1	
8.287E-01	1.095E+02	12.0	P059	1 1 1 0 1	
8.323E-01	1.100E+02	13	F300	1 0 0 0 1	
8.047E-01	1.063E+02	13.5	P059	1 1 1 0 1	
7.621E-01	1.007E+02	17.0	P059	1 1 1 0 1	
6.311E-01	8.341E+01	27.0	P059	1 1 1 0 1	
8.475E-01	1.120E+02	30	F300	1 0 0 0 2	
5.377E-01	7.106E+01	40.0	P059	1 1 1 0 1	
5.246E-01	6.933E+01	42.5	P059	1 1 1 0 1	
4.283E-01	5.660E+01	68.0	P059	1 1 1 0 1	
4.148E-01	5.482E+01	75.0	P059	1 1 1 0 1	
4.540E-01	6.000E+01	100	F300	1 0 0 0 0	

901. $C_6H_{12}O_3$
2-Ethoxyethyl acetate
Cellosolve acetate
RN: 111-15-9 **MP** (°C)**:** –61
MW: 132.16 **BP** (°C)**:** 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.499E+00	1.981E+02	20	D052	1 1 0 0 2	
1.415E+00	1.870E+02	20	M062	1 0 0 0 2	

902. $C_6H_{12}O_3$
Methyl β-ethoxypropionate
Methyl 3-ethoxypropionate
3-Ethoxypropionic acid methyl ester
RN: 14144-33-3 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.621E-01	1.007E+02	25	D002	1 2 1 1 2	
7.621E-01	1.007E+02	25	R034	0 0 0 0 2	

903. $C_6H_{12}O_5$
D-Quercitol
D-Quercit
RN: 488-73-3 **MP** (°C)**:** 234
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.701E-01	1.100E+02	20	F300	1 0 0 0 2	

904. $C_6H_{12}O_5$
Rhamnose
α-L-Rhamnose
6-Deoxy-L-mannose
L-Mannomethylose
L-Rhamnose
RN: 3615-41-6 **MP** (°C)**:** 82
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.212E+00	3.631E+02	18	D041	1 0 0 0 1	
3.177E+00	5.215E+02	40	D041	1 0 0 0 1	

905. $C_6H_{12}O_6$
D-Inositol
D(+)-Inositol
D-Chiro-inositol
(+)-Chiro-inositol
RN: 643-12-9 **MP** (°C)**:** 249.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	4.034E+02	11	F300	1 0 0 0 2	

906. $C_6H_{12}O_6$
D-Mannose
D-(+)-Mannose
Seminose
Carubinose
RN: 3458-28-4 **MP** (°C)**:** 132
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.956E+00	7.126E+02	17	D041	1 0 0 0 2	
3.957E+00	7.128E+02	17	F300	1 0 0 0 2	
2.399E+00	4.322E+02	25	G317	0 0 0 0 0	

907. $C_6H_{12}O_6$
Glucose
D-Glucose
D(+)-Glucose
Staleydex 111
Staleydex 333
RN: 50-99-7 **MP** (°C)**:** 146
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.954E+00	3.520E+02	.50	J019	1 0 1 2 2	
1.749E+00	3.151E+02	0	M043	1 0 0 0 1	
2.286E+00	4.118E+02	10	M043	1 0 0 0 1	
2.271E+00	4.091E+02	10.0	Y020	1 1 2 1 2	
3.365E+00	6.063E+02	15	D041	1 0 0 0 2	
2.660E+00	4.792E+02	20	M043	1 0 0 0 1	
2.314E+00	4.168E+02	20.0	Y020	1 1 2 1 2	
3.033E+00	5.464E+02	30	J019	1 0 1 2 2	
3.031E+00	5.460E+02	30	K122	1 1 1 1 2	
3.028E+00	5.455E+02	30	M043	1 0 0 0 2	
2.355E+00	4.244E+02	30.0	Y020	1 1 2 1 2	
1.901E+00	3.425E+02	30.50	M137	2 1 2 2 2	
2.042E+00	3.678E+02	35	B354	0 0 0 0 0	

(*continued*)

907. $C_6H_{12}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.416E+00	6.154E+02	40	M043	1 0 0 0 2	
2.396E+00	4.317E+02	40.0	Y020	1 1 2 1 2	
3.936E+00	7.091E+02	50	J019	1 0 1 2 2	
2.436E+00	4.388E+02	50.0	Y020	1 1 2 1 2	
4.090E+00	7.368E+02	60	M043	1 0 0 0 2	
4.005E+00	7.215E+02	70	A420	0 0 0 0 0	
4.523E+00	8.148E+02	80	M043	1 0 0 0 2	
2.227E+00	4.012E+02	.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	rt	D021	0 0 1 1 2	

908. $C_6H_{12}O_6$
Fructose
D-Fructose
D-(–)-Fructose
D-(–)-Levulose
Krystar 300
Nevulose
RN: 57-48-7 **MP** (°C)**:** 129
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	4.286E+02	0	M043	1 0 0 0 1	
4.318E+00	7.780E+02	20	F300	1 0 0 0 2	
2.467E+00	4.444E+02	20	M043	1 0 0 0 1	
4.524E+00	8.150E+02	30	K122	1 1 1 1 2	
4.524E+00	8.150E+02	30	K135	1 1 1 1 2	
2.448E+01	4.410E+03	30	K136	1 1 1 1 2	
2.550E+00	4.595E+02	40	M043	1 0 0 0 1	
2.629E+00	4.737E+02	60	M043	1 0 0 0 1	
4.709E+00	8.484E+02	70	A420	0 0 0 0 0	

909. $C_6H_{12}O_6$
Tagatose
Lyxo-2-hexulose
DL-Tagatose
RN: 17598-81-1 **MP** (°C)**:**
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.084E+00	3.755E+02	22	F300	1 0 0 0 2	

910. $C_6H_{12}O_6$
D-Galactose
Galactose
(+)-Galactose
D(+)-Galactose
RN: 59-23-4 **MP** (°C)**:** 169
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.046E-01	9.091E+01	0	D041	1 0 0 0 1	
2.247E+00	4.048E+02	25	D041	1 0 0 0 1	
2.253E+00	4.058E+02	rt	D021	0 0 1 1 2	

911. $C_6H_{12}O_6$
L-Sorbose
Sorbose
L-1,3,4,5,6-Pentahydroxyhexan-2-one
L-Xylo-2-hexulose
RN: 87-79-6 **MP** (°C)**:** 165
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.970E+00	3.548E+02	17	D041	1 0 0 0 1	
1.998E+00	3.600E+02	17	F300	1 0 0 0 1	

912. $C_6H_{12}O_6$
Inositol
Mesoinosit
cis-1,2,3,5-*trans*-4,6-Cyclohexanehexol
Dambose
Nucite
Phaseomannite
RN: 87-89-8 **MP** (°C)**:** 226
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.788E-01	1.403E+02	19	F300	1 0 0 0 2	
8.267E-01	1.489E+02	20	D041	1 0 0 0 2	
7.771E-01	1.400E+02	25	M054	1 0 0 0 1	
7.771E-01	1.400E+02	ns	L335	0 0 0 0 2	
7.762E-01	1.398E+02	ns	R424	0 0 0 0 0	

913. $C_6H_{12}O_6$
α-Glucose
α-D-Glucose
D-α-Glucose
Dextrose
RN: 492-62-6 **MP** (°C)**:** 154.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.355E+00	2.441E+02	0	D041	1 0 0 0 2	
2.019E+00	3.638E+02	10.0	Y020	1 1 2 1 2	
2.775E+00	5.000E+02	20	F300	1 0 0 0 0	
2.096E+00	3.775E+02	20.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	25	D041	1 0 0 0 2	
2.170E+00	3.909E+02	30.0	Y020	1 1 2 1 2	
2.242E+00	4.040E+02	40.0	Y020	1 1 2 1 2	
2.313E+00	4.168E+02	50.0	Y020	1 1 2 1 2	
2.346E+00	4.227E+02	54.7	Y020	1 1 2 1 2	
1.942E+00	3.498E+02	.0	Y020	1 1 2 1 2	

914. $C_6H_{12}O_6.H_2O$
Glucose (monohydrate)
RN: 50-99-7 **MP** (°C)**:** 83
MW: 198.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E+00	2.871E+02	10.0	Y020	1 1 2 1 2	
1.619E+00	3.209E+02	20.0	Y020	1 1 2 1 2	
1.781E+00	3.530E+02	30.0	Y020	1 1 2 1 2	
1.933E+00	3.831E+02	40.0	Y020	1 1 2 1 2	
2.072E+00	4.106E+02	50.0	Y020	1 1 2 1 2	
1.784E+00	3.536E+02	73.2	Y020	1 1 2 1 2	
1.274E+00	2.525E+02	.0	Y020	1 1 2 1 2	

915. $C_6H_{12}O_7$
Scyllitol
Scyllit
Quercinitol
Cocositol
RN: 488-59-5 **MP** (°C)**:** 253
MW: 196.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.149E-02	1.010E+01	18	F300	1 0 0 0 2	

916. $C_6H_{13}Br$

1-Bromohexane
Hexyl bromide

RN: 111-25-1 **MP** (°C)**:** –84.7
MW: 165.08 **BP** (°C)**:** 155.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-04	2.575E-02	25	M342	1 0 1 1 2	

917. $C_6H_{13}N$

1-Methylpiperidine
N-Methylpiperidine

RN: 626-67-5 **MP** (°C)**:** –18
MW: 99.18 **BP** (°C)**:** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+1.70E+00	+1.68E+02	ns	S460	0 0 0 0 0	

918. $C_6H_{13}NO$

Caproamide
n-Capronsaeure-amid
Hexanamide
Hexanoic acid, amide

RN: 628-02-4 **MP** (°C)**:** 99
MW: 115.18 **BP** (°C)**:** 255

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-01	1.854E+01	6	H059	0 0 0 0 0	
2.030E-01	2.338E+01	16	H059	0 0 0 0 0	
2.580E-01	2.972E+01	25	H059	0 0 0 0 0	
2.750E-01	3.167E+01	29	H059	0 0 0 0 0	
3.150E-01	3.628E+01	33	H059	0 0 0 0 0	
3.250E-01	3.743E+01	35	H059	0 0 0 0 0	
3.390E-01	3.904E+01	37	H059	0 0 0 0 0	
3.890E-01	4.480E+01	41	H059	0 0 0 0 0	

919. $C_6H_{13}NO_2$

L-Norleucine
Norleucine
α-Aminocaproic acid

RN: 327-57-1 **MP** (°C)**:** 327dec
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-01	1.710E+01	23	K060	1 2 0 0 2	
1.127E-01	1.478E+01	25	D041	1 0 0 0 1	
8.700E-02	1.141E+01	25	E015	1 2 1 1 1	
1.232E-01	1.616E+01	25	K031	2 1 2 1 2	

920. $C_6H_{13}NO_2$
L-Leucine
L(–)-Leucine
Leucine
2-Amino-4-methylpentanoic acid
L-2-Amino-4-methylpentanoic acid
(2*S*)-α-Leucine
RN: 61-90-5 **MP** (°C)**:** 286–288
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.692E-01	2.220E+01	0	F300	1 0 0 0 2	
1.740E-01	2.282E+01	15	D349	2 1 1 2 2	
1.601E-01	2.100E+01	20	B032	1 2 2 1 2	
1.800E-01	2.361E+01	20	D349	2 1 1 2 2	
1.695E-01	2.224E+01	21	P045	1 0 2 1 2	
1.772E-01	2.324E+01	24.99	C404	2 1 2 2 1	
1.640E-01	2.151E+01	25	B032	1 2 2 1 2	
1.712E-01	2.246E+01	25	C018	0 0 0 0 0	
1.851E-01	2.428E+01	25	C018	0 0 0 0 0	
1.700E-04	2.230E-02	25	C405	2 1 2 2 2	intrinsic zwit
1.883E-01	2.470E+01	25	D016	1 0 0 0 2	
1.634E-01	2.143E+01	25	D041	1 0 0 0 2	
1.860E-01	2.440E+01	25	D349	2 1 1 2 2	
1.807E-01	2.370E+01	25	F300	1 0 0 0 2	
1.626E-01	2.133E+01	25	G092	2 1 1 1 1	
1.626E-01	2.133E+01	25	G315	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N024	0 0 0 0 0	
1.654E-01	2.170E+01	25.1	N025	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N026	0 0 0 0 0	
1.612E-01	2.114E+01	25.1	N027	1 1 2 2 2	
1.765E-01	2.315E+01	27	D036	0 0 0 0 0	
1.601E-01	2.100E+01	27	D036	0 0 0 0 0	
1.682E-01	2.206E+01	29.80	B032	1 2 2 1 2	
1.907E-01	2.502E+01	34.99	C404	2 1 2 2 1	
2.041E-01	2.677E+01	44.99	C404	2 1 2 2 1	
2.142E-01	2.810E+01	50	F300	1 0 0 0 2	
2.805E-01	3.679E+01	75	D041	1 0 0 0 2	
2.805E-01	3.680E+01	75	F300	1 0 0 0 2	
2.886E-01	3.786E+01	92	M160	2 1 1 1 0	
4.071E-01	5.340E+01	100	F300	1 0 0 0 2	
4.069E-01	5.337E+01	99.99	P349	0 0 0 0 0	
1.830E-01	2.400E+01	ns	D072	0 0 0 0 1	

921. $C_6H_{13}NO_2$
L-*allo*-Isoleucine
Alloisoleucine
RN: 1509-34-8 **MP** (°C)**:** >280
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-01	2.818E+01	20	D041	1 0 0 0 1	

922. $C_6H_{13}NO_2$
D-Leucine
D-2-Amino-4-methylvaleric acid
D-2-Amino-4-methylpentanoic acid
RN: 328-38-1 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-01	2.153E+01	25	D041	1 0 0 0 2	
1.975E-01	2.591E+01	50	D041	1 0 0 0 2	

923. $C_6H_{13}NO_2$
D-Norleucine
D-2-Amino-*n*-caproic acid
D-2-Aminohexanoic acid
RN: 327-56-0 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.201E-01	1.575E+01	19	D041	1 0 0 0 1	

924. $C_6H_{13}NO_2$
tert-Amyl carbamate
tert-Pentyl carbamate
RN: 590-60-3 **MP** (°C)**:** 85
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-01	2.099E+01	37	H006	1 2 2 1 1	

925. $C_6H_{13}NO_2$
n-Amyl carbamate
n-Pentyl carbamate
O-Pentyl carbamate
RN: 638-42-6 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.460E+00	37	H006	1 2 2 1 1	

926. $C_6H_{13}NO_2$
Isopentyl urethane
Isoamylurethan
Isoamylurethane
RN: 543-86-2 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.660E-02	4.801E+00	15.5	F001	1 0 1 2 2	

927. $C_6H_{13}NO_2$
ε-Aminocaproic acid
6-Aminocaproic acid
ε-Amino-capronsaeure
RN: 60-32-2 **MP** (°C)**:** 205
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.848E+00	5.048E+02	25	M024	1 2 0 1 2	

928. $C_6H_{13}NO_2$
DL-Norleucine
DL-2-Amino-*n*-caproic acid
2-Aminohexanoic acid
DL-2-Aminohexanoic acid
RN: 616-06-8 **MP** (°C)**:** >300
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-02	9.003E+00	0	D018	2 2 2 1 2	
8.660E-02	1.136E+01	25	C018	0 0 0 0 0	
8.767E-02	1.150E+01	25	D016	1 0 0 0 2	
8.906E-02	1.168E+01	25	D018	2 2 2 1 2	
8.891E-02	1.166E+01	25	D041	1 0 0 0 2	
8.118E-02	1.065E+01	25	K031	2 1 2 1 2	
8.660E-02	1.136E+01	25	M024	1 2 0 1 2	
1.348E-01	1.768E+01	50	D018	2 2 2 1 2	
2.135E-01	2.800E+01	75	D018	2 2 2 1 2	
2.134E-01	2.799E+01	75	D041	1 0 0 0 2	
3.788E-01	4.969E+01	99.99	P349	0 0 0 0 0	

929. $C_6H_{13}NO_2$
L-Isoleucine
L(+)-Isoleucin
Isoleucine
RN: 73-32-5 **MP** (°C)**:** 288
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.844E-01	3.730E+01	15.50	F300	1 0 0 0 2	
2.533E-01	3.323E+01	20	B032	1 2 2 1 2	
2.619E-01	3.435E+01	25	B032	1 2 2 1 2	
3.017E-01	3.957E+01	25	D041	1 0 0 0 2	
2.458E-01	3.224E+01	25	G433	0 0 0 0 0	
2.364E-01	3.101E+01	25	O316	1 0 1 2 2	
2.358E-01	3.093E+01	25	O316	1 0 1 2 2	
2.714E-01	3.560E+01	27	D036	0 0 0 0 0	
2.690E-01	3.528E+01	29.80	B032	1 2 2 1 2	
4.369E-01	5.732E+01	75	D041	1 0 0 0 2	
3.801E-01	4.985E+01	84	M160	2 1 1 1 0	

930. $C_6H_{13}NO_2$
α-Hydroxycaproamide
Hexanamide, 2-hydroxy-
2-Hydroxyhexanamide
RN: 66461-73-2 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.300E-02	1.089E+01	25	M008	1 0 0 0 2	

931. $C_6H_{13}NO_2$
N-Propylurethane
Propylurethan
n-Propyl urethane
RN: 623-85-8 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.475E-01	9.805E+01	15.5	F001	1 0 1 2 2	

932. $C_6H_{13}NO_2$

DL-Isoleucine
DL-2-Amino-3-methylpentanoic acid
RN: 443-79-8 **MP** (°C)**:**
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-01	1.720E+01	0	D018	2 2 2 1 2	
1.632E-01	2.141E+01	25	D018	2 2 2 1 2	
1.662E-01	2.180E+01	25	D041	1 0 0 0 2	
2.235E-01	2.931E+01	50	D018	2 2 2 1 2	
3.510E-01	4.605E+01	75	D018	2 2 2 1 2	
3.357E-01	4.404E+01	75	D041	1 0 0 0 2	
5.517E-01	7.237E+01	99.99	P349	0 0 0 0 0	

933. $C_6H_{13}NO_2$

DL-Leucine
DL-2-Amino-4-methylvaleric acid
DL-2-Amino-4-methylpentanoic acid
RN: 328-39-2 **MP** (°C)**:** 295
MW: 131.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-02	8.735E+00	0	D018	2 2 2 1 2	
6.022E-02	7.900E+00	0	F300	1 0 0 0 1	
7.433E-02	9.750E+00	25	C018	0 0 0 0 0	
7.517E-02	9.860E+00	25	D016	1 0 0 0 2	
8.898E-02	1.167E+01	25	D018	2 2 2 1 2	
7.481E-02	9.813E+00	25	D041	1 0 0 0 2	
7.471E-02	9.800E+00	25	F300	1 0 0 0 1	
1.321E-01	1.733E+01	50	D018	2 2 2 1 2	
1.060E-01	1.390E+01	50	F300	1 0 0 0 2	
2.105E-01	2.762E+01	75	D018	2 2 2 1 2	
1.696E-01	2.225E+01	75	D041	1 0 0 0 2	
1.700E-01	2.230E+01	75	F300	1 0 0 0 2	
3.080E-01	4.040E+01	100	F300	1 0 0 0 2	
3.077E-01	4.036E+01	99.99	P349	0 0 0 0 0	
7.324E-02	9.607E+00	rt	H431	0 0 0 0 0	average

934. C_6H_{14}

Hexane
Normal hexane
n-Hexane
Skellysolve B
RN: 110-54-3 **MP** (°C)**:** –95
MW: 86.18 **BP** (°C)**:** 65

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-04	1.650E-02	0	P003	2 2 2 2 2	
1.900E-04	1.637E-02	4.0	N004	1 1 2 2 2	

(*continued*)

934. C_6H_{14} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-04	1.518E-02	14.0	N004	1 1 2 2 2	
1.600E-03	1.379E-01	15.5	F001	1 0 1 0 2	
6.382E-04	5.500E-02	16	D047	1 0 0 1 1	
1.427E-04	1.230E-02	25	A058	1 1 1 1 2	
1.624E-03	1.400E-01	25	A094	1 0 0 0 1	
1.625E-03	1.400E-01	25	K072	1 0 1 1 1	
1.857E-03	1.600E-01	25	K112	1 0 2 1 1	
1.860E-03	1.603E-01	25	K112	1 0 2 2 2	
1.099E-04	9.470E-03	25	K119	1 0 0 0 2	
1.427E-04	1.230E-02	25	L002	2 2 2 2 2	
1.102E-04	9.500E-03	25	M001	2 1 2 2 2	
1.102E-04	9.500E-03	25	M002	2 1 2 2 2	
1.102E-04	9.500E-03	25	M040	1 0 0 1 1	
1.625E-03v	1.400E-01	25	M087	1 1 2 1 1	
1.430E-04	1.232E-02	25	M342	1 0 1 1 2	
1.439E-04	1.240E-02	25	P003	2 2 2 2 2	
1.624E-03	1.400E-01	25	S012	2 0 2 2 1	
2.128E-04	1.834E-02	25.0	N004	1 1 2 2 2	
1.099E-04	9.470E-03	25.0	P051	2 1 1 2 2	
1.099E-04	9.470E-03	25.00	P007	2 1 2 2 2	
1.494E-04	1.288E-02	35.0	N004	1 1 2 2 2	
4.623E-02	3.984E+00	38	J020	2 0 2 1 0	*sic*
1.172E-04	1.010E-02	40.1	P051	2 1 1 2 2	
1.172E-04	1.010E-02	40.10	P007	2 1 2 2 2	
2.578E-04	2.221E-02	45.0	N004	1 1 2 2 2	
2.553E-03	2.200E-01	50	L097	1 1 1 1 1	
2.456E-04	2.116E-02	55.0	N004	1 1 2 2 2	
1.532E-04	1.320E-02	55.7	P051	2 1 1 2 2	
1.532E-04	1.320E-02	55.70	P007	2 1 2 2 2	
1.775E-04	1.530E-02	69.7	P051	2 1 1 2 2	average of 2
1.764E-04	1.520E-02	69.70	P007	2 1 2 2 2	
1.787E-04	1.540E-02	69.70	P007	2 1 2 2 2	
2.599E-04	2.240E-02	99.1	P051	2 1 1 2 2	
2.599E-04	2.240E-02	99.10	P007	2 1 2 2 2	
3.388E-04	2.920E-02	114.4	P051	2 1 1 2 2	
3.388E-04	2.920E-02	114.40	P007	2 1 2 2 2	
4.363E-04	3.760E-02	121.3	P051	2 1 1 2 2	
4.363E-04	3.760E-02	121.30	P007	2 1 2 2 2	
6.603E-04	5.690E-02	137.3	P051	2 1 1 2 2	
6.603E-04	5.690E-02	137.30	P007	2 1 2 2 2	
1.230E-03	1.060E-01	151.8	P051	2 1 1 2 2	
1.230E-03	1.060E-01	151.80	P007	2 1 2 2 2	
1.102E-04	9.500E-03	ns	H123	0 0 0 0 0	
1.392E-03	1.200E-01	ns	M010	0 0 0 0 1	
1.880E-04	1.620E-02	ns	M175	0 0 2 1 2	

935. C_6H_{14}

2,2-Dimethylbutane
Neohexane

RN: 75-83-2 **MP** (°C)**:** –100
MW: 86.18 **BP** (°C)**:** 50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.572E-04	3.940E-02	0	P003	2 2 2 2 2	
4.278E-04	3.686E-02	2.34	S461	0 0 0 0 0	
3.444E-04	2.968E-02	9.99	S461	0 0 0 0 0	
2.722E-04	2.346E-02	24.99	S461	0 0 0 0 0	
2.460E-04	2.120E-02	25	K119	1 0 0 0 2	
2.135E-04	1.840E-02	25	M001	2 1 2 2 2	
2.135E-04	1.840E-02	25	M002	2 1 2 2 2	
2.762E-04	2.380E-02	25	P003	2 2 2 2 2	
2.460E-04	2.120E-02	25	P051	2 1 1 2 2	
2.460E-04	2.120E-02	25.00	P007	2 1 2 2 2	
6.600E-04	5.687E-02	ns	J300	0 0 0 0 0	

936. C_6H_{14}

2,3-Dimethylbutane
Diisopropyl
1,1,2,2-Tetramethylethane

RN: 79-29-8 **MP** (°C)**:** –129
MW: 86.18 **BP** (°C)**:** 58

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.818E-04	3.290E-02	0	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25	K119	1 0 0 0 2	
2.611E-04	2.250E-02	25	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25.0	P051	2 1 1 2 2	
2.216E-04	1.910E-02	25.00	P007	2 1 2 2 2	
2.228E-04	1.920E-02	40.1	P051	2 1 1 2 2	
2.228E-04	1.920E-02	40.10	P007	2 1 2 2 2	
2.750E-04	2.370E-02	55.1	P051	2 1 1 2 2	
2.750E-04	2.370E-02	55.10	P007	2 1 2 2 2	
4.653E-04	4.010E-02	99.1	P051	2 1 1 2 2	
4.653E-04	4.010E-02	99.10	P007	2 1 2 2 2	
6.591E-04	5.680E-02	121.3	P051	2 1 1 2 2	
6.591E-04	5.680E-02	121.30	P007	2 1 2 2 2	
1.136E-03	9.790E-02	137.3	P051	2 1 1 2 2	
1.136E-03	9.790E-02	137.30	P007	2 1 2 2 2	
1.984E-03	1.710E-01	149.5	P051	2 1 1 2 2	
1.984E-03	1.710E-01	149.50	P007	2 1 2 2 2	

937. C_6H_{14}
2-Methylpentane
2-Metylopentan
RN: 107-83-5 **MP** (°C)**:** –154
MW: 86.18 **BP** (°C)**:** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.257E-04	1.945E-02	0	P003	2 2 2 2 2	
5.976E-04	5.150E-02	23	C332	0 0 0 0 0	
1.508E-04	1.300E-02	25	K119	1 0 0 0 2	
1.648E-04	1.420E-02	25	L002	2 2 2 2 2	
1.601E-04	1.380E-02	25	M001	2 1 2 2 2	
1.601E-04	1.380E-02	25	M002	2 1 2 2 2	
1.822E-04	1.570E-02	25	P003	2 2 2 2 2	
1.508E-04	1.300E-02	25.0	P051	2 1 1 2 2	
1.508E-04	1.300E-02	25.00	P007	2 1 2 2 2	
1.601E-04	1.380E-02	40.1	P051	2 1 1 2 2	
1.601E-04	1.380E-02	40.10	P007	2 1 2 2 2	
1.822E-04	1.570E-02	55.7	P051	2 1 1 2 2	
1.822E-04	1.570E-02	55.70	P007	2 1 2 2 2	
3.145E-04	2.710E-02	99.1	P051	2 1 1 2 2	
3.145E-04	2.710E-02	99.10	P007	2 1 2 2 2	
5.210E-04	4.490E-02	118.0	P051	2 1 1 2 2	
5.210E-04	4.490E-02	118.00	P007	2 1 2 2 2	
1.007E-03	8.680E-02	137.3	P051	2 1 1 2 2	
1.007E-03	8.680E-02	137.30	P007	2 1 2 2 2	
1.311E-03	1.130E-01	149.50	P007	2 1 2 2 2	

938. C_6H_{14}
3-Methylpentane
3-Metylopentan
RN: 96-14-0 **MP** (°C)**:** –118
MW: 86.18 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-04	2.150E-02	0	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	K119	1 0 0 0 2	
1.485E-04	1.280E-02	25	M001	2 1 2 2 2	
2.077E-04	1.790E-02	25	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	P051	2 1 1 2 2	
1.520E-04	1.310E-02	25.00	P007	2 1 2 2 2	
1.485E-04	1.280E-02	ns	H123	0 0 0 0 0	

939. $C_6H_{14}FO_3P$
Isofluorphate
Diisopropylfluorophosphate
Phosphorofluoridic acid bis(1-methylethyl) ester
Difluorophate
PF-3
T-1703
RN: 55-91-4 **MP** (°C)**:** –82
MW: 184.15 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.236E-02	1.517E+01	25	D041	1 0 0 0 2	

940. $C_6H_{14}NO_3PS_2$
Ethoate-methyl
O,*O*-Dimethyl *S*-(*N*-ethylcarbamoylmethyl) dithiophosphate
Fitios
RN: 116-01-8 **MP** (°C)**:** 66.1
MW: 243.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-02	8.500E+00	25	M061	1 0 0 0 1	
3.494E-02	8.500E+00	25	M161	1 0 0 0 1	

941. $C_6H_{14}N_2$
trans-2,5-Dimethylpiperazine
trans-2,5-Dimethyl-piperazin
RN: 2815-34-1 **MP** (°C)**:**
MW: 114.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.065E+00	3.500E+02	20	F300	1 0 0 0 1	

942. $C_6H_{14}N_2O$
Methyl-*n*-amylnitrosamine
N-Nitroso(methyl)pentylamine
RN: 13256-07-0 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-02	1.094E+01	24	D083	2 0 0 0 1	

943. $C_6H_{14}N_2O$
Di-*n*-propylnitrosamine
N-Nitroso-*N*-propyl-1-propanamine
Dipropylnitrosamine
NDPA
DPNA
Nitrosodipropylamine
RN: 621-64-7 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	9.895E+00	24	D083	2 0 0 0 1	

944. $C_6H_{14}N_2O$
Ethyl-*n*-butylnitrosamine
Nitroso-*N*-ethyl-*n*-butylamine
N-Nitroso-*N*-butylethylamine
N-Nitroso(ethyl)-*n*-butylamine
NEBA
Butanamine, *N*-ethyl-*N*-nitroso-
RN: 4549-44-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-02	1.198E+01	24	D083	2 0 0 0 1	

945. $C_6H_{14}N_2O$
Di-isopropylnitrosamine
2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso-
N-Nitrosodiisopropylamine
NdiPA
RN: 601-77-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.302E+01	24	D083	2 0 0 0 1	

946. $C_6H_{14}N_2O_2$
L(+)-Lysine
L(+)-Lysin
Lysine
RN: 56-87-1 **MP** (°C)**:** 224
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.995E+00	5.840E+02	27	D036	0 0 0 0 0	

947. $C_6H_{14}N_4O_2$
DL-Arginine
(±)-Arginine
RN: 7200-25-1 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.382E+00	2.407E+02	20	J303	0 0 0 0 0	
1.978E+00	3.445E+02	40	J303	0 0 0 0 0	
2.781E+00	4.844E+02	50	J303	0 0 0 0 0	
3.851E+00	6.709E+02	60	J303	0 0 0 0 0	

948. $C_6H_{14}N_4O_2$
L-Arginine
L(+)-Arginin
Arginine
RN: 74-79-3 **MP** (°C)**:** 244
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.559E-01	1.143E+02	10	H062	1 2 2 0 0	EFG
8.588E-01	1.496E+02	20	B032	1 2 2 1 2	
7.487E-01	1.304E+02	21	D041	1 0 0 0 1	
8.037E-01	1.400E+02	21	F300	1 0 0 0 0	average
1.044E+00	1.818E+02	25	B032	1 2 2 1 2	
9.230E-01	1.608E+02	25	G315	0 0 0 0 0	
3.060E+00	5.330E+02	27	D036	0 0 0 0 0	
1.241E+00	2.162E+02	29.80	B032	1 2 2 1 2	
1.111E+00	1.935E+02	30	H062	1 2 2 0 0	EFG
1.771E+00	3.084E+02	50	H062	1 2 2 0 0	EFG

949. $C_6H_{14}O$
3-Methyl-3-pentanol
Diethylmethylcarbinol
RN: 77-74-7 **MP** (°C)**:** –24
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-01	4.379E+01	9.8	S307	1 1 0 2 2	
3.346E-01	3.419E+01	19.5	S307	1 1 0 2 2	
4.500E-01	4.598E+01	20	G005	1 2 1 1 2	
3.999E-01	4.086E+01	25	G005	1 2 1 1 2	
3.264E-01	3.335E+01	29.8	S307	1 1 0 2 2	
3.592E-01	3.670E+01	30	G005	1 2 1 1 2	
2.647E-01	2.705E+01	39.8	S307	1 1 0 2 2	
2.331E-01	2.382E+01	49.7	S307	1 1 0 2 2	
1.938E-01	1.980E+01	59.5	S307	1 1 0 2 2	
1.834E-01	1.874E+01	70.1	S307	1 1 0 2 2	
1.787E-01	1.826E+01	80.1	S307	1 1 0 2 2	
1.617E-01	1.652E+01	90.4	S307	1 1 0 2 2	

950. $C_6H_{14}O$
Dipropyl ether
Propyl ether
Dipropylaether
Dipropylether
RN: 111-43-3 **MP** (°C)**:** –123
MW: 102.18 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.644E-02	5.767E+00	0	B002	2 1 1 2 2	
3.996E-02	4.083E+00	10	B002	2 1 1 2 2	
3.705E-02	3.786E+00	15	B002	2 1 1 2 2	
2.927E-02	2.991E+00	20	B002	2 1 1 2 2	
2.936E-02	3.000E+00	20	F300	1 0 0 0 0	
6.700E-02	6.846E+00	20	S006	1 0 0 0 1	
2.441E-02	2.494E+00	25	B002	2 1 1 2 2	
1.070E-01	1.093E+01	37	E028	1 0 1 1 2	

951. $C_6H_{14}O$
tert-Amyl methyl ether
Methyl *tert*-amyl ether
RN: 994-05-8 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-01	1.235E+01	20	E019	1 0 1 1 2	

952. $C_6H_{14}O$
Propyl isopropyl ether
Propyl-isopropyl-aether
RN: 627-08-7 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.285E-02	7.444E+00	10	B002	2 1 1 2 2	
7.242E-02	7.400E+00	10	F300	1 0 0 0 1	
5.837E-02	5.964E+00	15	B002	2 1 1 2 2	
5.872E-02	6.000E+00	15	F300	1 0 0 0 1	
4.966E-02	5.074E+00	20	B002	2 1 1 2 2	
4.578E-02	4.678E+00	25	B002	2 1 1 2 2	
4.600E-02	4.700E+00	25	F300	1 0 0 0 1	

953. $C_6H_{14}O$
Isohexyl alcohol
4-Methyl-1-pentanol
RN: 626-89-1 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-01	1.042E+01	20	H330	0 0 0 0 0	

954. $C_6H_{14}O$
4-Methyl-2-pentanol
i-Butylmethylcarbinol
Methyl amyl alcohol
RN: 108-11-2 **MP** (°C)**:** –90
MW: 102.18 **BP** (°C)**:** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.684E-01	2.743E+01	0	S307	1 1 0 2 2	
2.004E-01	2.047E+01	9.7	S307	1 1 0 2 2	
1.664E-01	1.701E+01	20	D052	1 1 0 0 2	
1.721E-01	1.759E+01	20	G005	1 2 1 1 2	
1.570E-01	1.604E+01	20.0	S307	1 1 0 2 2	
1.636E-01	1.672E+01	25	C093	2 1 1 1 1	
1.579E-01	1.614E+01	25	G005	1 2 1 1 2	
1.465E-01	1.497E+01	30	G005	1 2 1 1 2	
1.475E-01	1.507E+01	30.0	S307	1 1 0 2 2	
1.246E-01	1.274E+01	40.3	S307	1 1 0 2 2	
1.151E-01	1.176E+01	50.0	S307	1 1 0 2 2	
1.074E-01	1.098E+01	60.1	S307	1 1 0 2 2	
1.094E-01	1.117E+01	70.2	S307	1 1 0 2 2	
1.199E-01	1.225E+01	80.2	S307	1 1 0 2 2	
1.132E-01	1.156E+01	90.2	S307	1 1 0 2 2	

955. $C_6H_{14}O$
2,2-Dimethyl-3-butanol
t-Butylmethylcarbinol
RN: 464-07-3 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.517E-01	2.572E+01	20	G005	1 2 1 1 2	
2.322E-01	2.372E+01	25	G005	1 2 1 1 2	
2.163E-01	2.210E+01	30	G005	1 2 1 1 2	

956. $C_6H_{14}O$
1-Hexanol
n-Hexanol
Amyl carbinol
Caproic alcohol
n-Hexyl alcohol
RN: 111-27-3 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.173E-01	2.220E+01	0	C423	0 0 0 0 0	
7.864E-02	8.035E+00	0	E029	1 2 0 1 1	
9.344E-02	9.548E+00	0	S307	1 1 0 2 2	
1.732E-01	1.770E+01	4	C423	0 0 0 0 0	
7.706E-02	7.873E+00	5.54	H110	2 2 2 2 2	
7.487E-02	7.650E+00	6.84	H110	2 2 2 2 2	
7.213E-02	7.370E+00	8.64	H110	2 2 2 2 2	
1.223E-01	1.250E+01	10	C423	0 0 0 0 0	
6.803E-02	6.951E+00	10	E029	1 2 0 1 1	
7.372E-02	7.533E+00	10.2	S307	1 1 0 2 2	
6.906E-02	7.057E+00	11.04	H110	2 2 2 2 2	
6.671E-02	6.816E+00	12.94	H110	2 2 2 2 2	
6.506E-02	6.648E+00	14.64	H110	2 2 2 2 2	
6.287E-02	6.424E+00	17.04	H110	2 2 2 2 2	
6.861E-02	7.011E+00	20	A015	1 2 1 1 2	
6.224E-02	6.359E+00	20	E029	1 2 0 1 1	
6.070E-02	6.202E+00	20	H330	0 0 0 0 0	
4.869E-02	4.975E+00	20	L049	1 1 2 1 0	
5.150E-02	5.262E+00	20	P073	1 0 0 1 2	
6.475E-02	6.616E+00	20.0	S307	1 1 0 2 2	
5.991E-02	6.121E+00	20.74	H110	2 2 2 2 2	
5.854E-02	5.981E+00	22.94	H110	2 2 2 2 2	
6.250E-02	6.386E+00	24	H345	0 0 0 0 0	
6.069E-02	6.201E+00	25	B038	1 2 1 1 2	
5.644E-02	5.767E+00	25	B060	2 0 1 1 1	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.047E-02	7.200E+00	25	C435	0 0 0 0 0	
1.000E+00	1.022E+02	25	F044	1 0 0 0 0	EFG
8.000E-02	8.174E+00	25	G075	1 0 1 0 0	
5.900E-02	6.028E+00	25	K025	2 2 1 1 2	
8.922E-02	9.116E+00	25	M323	2 2 1 1 2	
5.711E-02	5.835E+00	25.04	H110	2 2 2 2 2	
5.640E-02	5.762E+00	26.94	H110	2 2 2 2 2	
5.579E-02	5.701E+00	28.94	H110	2 2 2 2 2	
5.431E-02	5.549E+00	29.7	S307	1 1 0 2 2	
6.320E-02	6.458E+00	30	C091	1 2 1 1 1	
5.740E-02	5.865E+00	30	E029	1 2 0 1 1	
5.517E-02	5.637E+00	30.94	H110	2 2 2 2 2	
5.440E-02	5.558E+00	33.04	H110	2 2 2 2 2	
5.005E-02	5.114E+00	39.8	S307	1 1 0 2 2	
5.257E-02	5.371E+00	40	E029	1 2 0 1 1	

(*continued*)

956. $C_6H_{14}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.869E-02	4.975E+00	50	E029	1 2 0 1 1	
4.840E-02	4.945E+00	50.0	S307	1 1 0 2 2	
5.063E-02	5.173E+00	60	E029	1 2 0 1 1	
5.043E-02	5.153E+00	60.0	S307	1 1 0 2 2	
5.450E-02	5.569E+00	70	E029	1 2 0 1 1	
5.540E-02	5.661E+00	70	F001	1 0 1 0 2	
5.615E-02	5.737E+00	70.3	S307	1 1 0 2 2	
5.934E-02	6.063E+00	80	E029	1 2 0 1 1	
6.080E-02	6.212E+00	80	F001	1 0 1 0 2	
6.079E-02	6.211E+00	80.3	S307	1 1 0 2 2	
6.707E-02	6.853E+00	90	E029	1 2 0 1 1	
6.660E-02	6.805E+00	90	F001	1 0 1 0 2	
6.204E-02	6.340E+00	90.3	S307	1 1 0 2 2	
7.767E-02	7.937E+00	100	E029	1 2 0 1 1	
7.690E-02	7.857E+00	100	F001	1 0 1 0 2	
8.826E-02	9.018E+00	110	E029	1 2 0 1 1	
8.720E-02	8.910E+00	110	F001	1 0 1 0 2	
1.007E-01	1.029E+01	120	E029	1 2 0 1 2	
1.151E-01	1.176E+01	130	E029	1 2 0 1 2	
1.323E-01	1.351E+01	140	E029	1 2 0 1 2	
1.570E-01	1.604E+01	150	E029	1 2 0 1 2	
1.966E-01	2.009E+01	160	E029	1 2 0 1 2	
2.573E-01	2.629E+01	170	E029	1 2 0 1 2	
3.410E-01	3.484E+01	180	E029	1 2 0 1 2	
4.545E-01	4.644E+01	190	E029	1 2 0 1 2	
6.188E-01	6.323E+01	200	E029	1 2 0 1 2	
8.654E-01	8.842E+01	210	E029	1 2 0 1 2	
1.372E+00	1.402E+02	220	E029	1 2 0 1 2	
6.114E-02	6.247E+00	ns	L003	0 0 2 1 2	

957. $C_6H_{14}O$

2-Hexanol
n-Butylmethylcarbinol
1-Methyl pentanol

RN: 626-93-7 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.975E-01	2.018E+01	0	S307	1 1 0 2 2	
1.617E-01	1.652E+01	10.1	S307	1 1 0 2 2	
1.246E-01	1.274E+01	19.8	S307	1 1 0 2 2	
1.456E-01	1.488E+01	20	G005	1 2 1 1 2	
1.690E-01	1.727E+01	20	H330	0 0 0 0 0	
1.323E-01	1.351E+01	25	G005	1 2 1 1 2	
1.141E-01	1.166E+01	29.9	S307	1 1 0 2 2	
1.237E-01	1.264E+01	30	G005	1 2 1 1 2	
1.055E-01	1.078E+01	40.0	S307	1 1 0 2 2	
9.306E-02	9.509E+00	50.0	S307	1 1 0 2 2	

(*continued*)

957. $C_6H_{14}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.826E-02	9.018E+00	60.2	S307	1 1 0 2 2	
9.498E-02	9.705E+00	70.0	S307	1 1 0 2 2	
1.094E-01	1.117E+01	80.1	S307	1 1 0 2 2	
9.114E-02	9.312E+00	90.2	S307	1 1 0 2 2	

958. $C_6H_{14}O$

2,2-Dimethyl-1-butanol
t-Pentylcarbinol
RN: 1185-33-7 **MP** (°C)**:** –35
MW: 102.18 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.960E-02	8.133E+00	20	G005	1 2 1 1 1	
7.382E-02	7.543E+00	25	G005	1 2 1 1 1	
6.900E-02	7.050E+00	30	G005	1 2 1 1 1	

959. $C_6H_{14}O$

2,3-Dimethyl-1-butanol
Dimethyl-*i*-propylcarbinol
Dimethyl-isopropylcarbinol
RN: 594-60-5 **MP** (°C)**:** –14
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.349E-01	4.443E+01	20	G005	1 2 1 1 2	
3.927E-01	4.012E+01	25	G005	1 2 1 1 2	
3.547E-01	3.624E+01	30	G005	1 2 1 1 2	

960. $C_6H_{14}O$

Isopropyl ether
Diisopropyl ether
RN: 108-20-3 **MP** (°C)**:** –60
MW: 102.18 **BP** (°C)**:** 68.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E-01	1.381E+01	24.6	H121	2 0 0 0 1	
8.730E-02	8.920E+00	25	F048	2 0 0 0 0	
7.920E-02	8.092E+00	37	E028	1 0 1 1 2	

961. $C_6H_{14}O$
2-Ethyl-1-butanol
2-Ethylbutanol
RN: 97-95-0 **MP** (°C)**:** –15
MW: 102.18 **BP** (°C)**:** 146

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.127E-02	6.261E+00	20	D052	1 1 0 0 1	
3.899E-02	3.984E+00	25	C093	2 1 1 1 0	

962. $C_6H_{14}O$
3-Methyl-2-pentanol
3-Methyl-2-pentyl alcohol
RN: 565-60-6 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.004E-01	2.047E+01	20	G005	1 2 1 1 2	
1.863E-01	1.903E+01	25	G005	1 2 1 1 2	
1.721E-01	1.759E+01	30	G005	1 2 1 1 2	

963. $C_6H_{14}O$
2-Ethyl-4-butanol
3-Methylpentanol
RN: 105-30-6 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.284E+01	0	S307	1 1 0 2 2	
1.004E-01	1.025E+01	10.0	S307	1 1 0 2 2	
8.518E-02	8.704E+00	19.6	S307	1 1 0 2 2	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.681E-02	7.848E+00	30.8	S307	1 1 0 2 2	
7.498E-02	7.661E+00	40.3	S307	1 1 0 2 2	
7.295E-02	7.454E+00	50.0	S307	1 1 0 2 2	
7.363E-02	7.523E+00	60.3	S307	1 1 0 2 2	
7.478E-02	7.641E+00	70.1	S307	1 1 0 2 2	
8.133E-02	8.310E+00	80.3	S307	1 1 0 2 2	
8.931E-02	9.126E+00	90.7	S307	1 1 0 2 2	

964. $C_6H_{14}O$

2-Methyl-2-pentanol
Dimethyl-*n*-propylcarbinol
1,1-Dimethyl-1-butanol

RN: 590-36-3 **MP** (°C)**:** –107
MW: 102.18 **BP** (°C)**:** 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.428E-01	3.503E+01	20	G005	1 2 1 1 2	
3.640E-01	3.719E+01	20	H330	0 0 0 0 0	
3.071E-01	3.138E+01	25	G005	1 2 1 1 2	
2.814E-01	2.875E+01	30	G005	1 2 1 1 2	

965. $C_6H_{14}O$

2-Methyl-3-pentanol
i-Propylethylcarbinol

RN: 565-67-3 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.144E-01	2.191E+01	20	G005	1 2 0 0 2	
1.928E-01	1.970E+01	25	G005	1 2 1 1 2	
1.749E-01	1.787E+01	30	G005	1 2 1 1 2	

966. $C_6H_{14}O$

3-Hexanol
n-Propylethylcarbinol
tert-Hexyl alcohol

RN: 623-37-0 **MP** (°C)**:** <25
MW: 102.18 **BP** (°C)**:** 134.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E-01	2.676E+01	0	S307	1 1 0 2 2	
1.881E-01	1.922E+01	10.1	S307	1 1 0 2 2	
3.062E-01	3.129E+01	20	A015	1 2 1 1 2	
1.683E-01	1.720E+01	20	G005	1 2 1 1 2	
1.608E-01	1.643E+01	20.0	S307	1 1 0 2 2	
1.551E-01	1.584E+01	25	G005	1 2 1 1 2	
1.437E-01	1.468E+01	30	G005	1 2 1 1 2	
1.342E-01	1.371E+01	30.0	S307	1 1 0 2 2	
1.189E-01	1.215E+01	39.8	S307	1 1 0 2 2	
1.065E-01	1.088E+01	50.0	S307	1 1 0 2 2	
9.882E-02	1.010E+01	60.1	S307	1 1 0 2 2	
9.882E-02	1.010E+01	70.2	S307	1 1 0 2 2	
1.036E-01	1.059E+01	80.2	S307	1 1 0 2 2	
1.065E-01	1.088E+01	90.3	S307	1 1 0 2 2	

967. $C_6H_{14}O$
3-Methyl-1-pentanol
3-Methylpentanol
2-Ethyl-4-butanol
RN: 589-35-5 **MP** (°C)**:**
MW: 102.18 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.190E-02	4.282E+00	25	B060	2 0 1 1 1	

968. $C_6H_{14}O_2$
Acetal
Acetaldehyd-diaethylacetal
Acetaldehyde diethyl acetal
RN: 105-57-7 **MP** (°C)**:**
MW: 118.18 **BP** (°C)**:** 102.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.723E-01	4.400E+01	25	F300	1 0 0 0 1	

969. $C_6H_{14}O_2$
Diethyl cellosolve
Ethylene glycol diethyl ether
1,2-Diethoxyethane
3,6-Dioxaoctane
Ethyl glyme
Diethoxyethane
RN: 629-14-1 **MP** (°C)**:**
MW: 118.18 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.273E-01	2.686E+01	20	D052	1 1 0 0 2	
1.469E+00	1.736E+02	20	M062	1 0 0 0 2	

970. $C_6H_{14}O_3$
Carbitol
2-(2-Ethoxyethoxy)ethanol
RN: 111-90-0 **MP** (°C)**:**
MW: 134.18 **BP** (°C)**:** 196.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E+00	4.843E+02	4.50	C022	1 2 0 0 2	

971. $C_6H_{14}O_6$
D-Mannitol
1,2,3,4,5,6-Hexanehexol
Cordycepic acid
Diosmol
D-Mannite
Manna sugar
RN: 69-65-8 **MP** (°C)**:** 167–170
MW: 182.17 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E+00	2.092E+02	ns	R427	0 0 0 0 0	

972. $C_6H_{14}O_6$
Galactitol
Dulcit
Dulcitol
RN: 608-66-2 **MP** (°C)**:** 189.5
MW: 182.17 **BP** (°C)**:** 277.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.599E-01	2.913E+01	14	D041	1 0 0 0 1	
1.702E-01	3.100E+01	15	F300	1 0 0 0 1	
2.086E+00	3.800E+02	100	F300	1 0 0 0 1	

973. $C_6H_{14}O_6$
Sorbitol
D-Sorbitol
RN: 50-70-4 **MP** (°C)**:** 110
MW: 182.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E+00	6.416E+02	10	M043	1 0 0 0 2	
3.785E+00	6.894E+02	20	M043	1 0 0 0 2	
4.025E+00	7.333E+02	30	M043	1 0 0 0 2	
4.283E+00	7.802E+02	40	M043	1 0 0 0 2	

974. $C_6H_{14}O_6$
Mannitol
D-Mannit
D-Mannitol
RN: 87-78-5 **MP** (°C)**:** 167
MW: 182.17 **BP** (°C)**:** 292

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.081E-01	9.256E+01	0	C073	1 2 2 1 2	
5.171E-01	9.420E+01	0	M043	1 0 0 0 2	

(*continued*)

974. $C_6H_{14}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-01	1.205E+02	10	M043	1 0 0 0 2	
7.734E-01	1.409E+02	15	C073	1 2 2 1 2	
7.740E-01	1.410E+02	15	F300	1 0 0 0 2	
7.408E-01	1.349E+02	18	D041	1 0 0 0 2	
7.936E-01	1.446E+02	19	N051	1 0 2 2 2	
8.609E-01	1.568E+02	20	M043	1 0 0 0 2	
7.571E-01	1.379E+02	21.6	Y412	0 0 0 0 0	
9.762E-01	1.778E+02	25	B106	1 2 2 2 2	
9.732E-01	1.773E+02	25	B106	1 2 2 2 2	
9.739E-01	1.774E+02	25	B106	1 2 2 2 2	
9.639E-01	1.756E+02	25	C073	1 2 2 1 2	
8.255E-01	1.504E+02	25	H087	1 0 2 1 2	
8.373E-01	1.525E+02	26.8	Y412	0 0 0 0 0	
1.000E+00	1.822E+02	30	D011	1 0 1 0 1	
1.105E+00	2.013E+02	30	M043	1 0 0 0 2	
9.149E-01	1.667E+02	30.8	Y412	0 0 0 0 0	
1.254E+00	2.284E+02	35	C073	1 2 2 1 2	
9.899E-01	1.803E+02	35.6	Y412	0 0 0 0 0	
1.062E+00	1.935E+02	38.1	Y412	0 0 0 0 0	
1.411E+00	2.571E+02	40	M043	1 0 0 0 2	
1.133E+00	2.063E+02	41.8	Y412	0 0 0 0 0	
1.760E+00	3.207E+02	50	C073	1 2 2 1 2	
1.827E+00	3.329E+02	51.50	B106	1 2 2 2 2	
2.083E+00	3.794E+02	60	C073	1 2 2 1 2	
2.104E+00	3.833E+02	60	F300	1 0 0 0 2	
2.150E+00	3.917E+02	60	M043	1 0 0 0 2	
2.416E+00	4.401E+02	67.40	B106	1 2 2 2 2	
2.504E+00	4.562E+02	70.50	B106	1 2 2 2 2	
2.936E+00	5.349E+02	80	M043	1 0 0 0 2	
3.015E+00	5.493E+02	82.90	B106	1 2 2 2 2	
3.253E+00	5.927E+02	88.10	B106	1 2 2 2 2	
3.299E+00	6.010E+02	90.10	B106	1 2 2 2 2	
3.590E+00	6.540E+02	98	B106	1 2 2 2 2	
3.628E+00	6.610E+02	99.30	B106	1 2 2 2 2	
3.641E+00	6.633E+02	100	M043	1 0 0 0 2	
8.757E-01	1.595E+02	rt	D021	0 0 1 1 2	

975. $C_6H_{15}N$

Triethylamine
Triaethylamin

RN: 121-44-8 **MP** (°C)**:** –115
MW: 101.19 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E+00	1.799E+02	17.48	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.59	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.64	K142	1 0 0 0 2	

(*continued*)

975. $C_6H_{15}N$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.156E+00	1.170E+02	17.82	K142	1 0 0 0 2	
1.156E+00	1.170E+02	17.85	K142	1 0 0 0 2	
2.791E+00	2.824E+02	18	C088	2 2 2 2 1	
3.434E+00	3.475E+02	18.11	K142	1 0 0 0 2	
3.434E+00	3.475E+02	18.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.13	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.38	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.43	K142	1 0 0 0 2	
1.403E+00	1.420E+02	20	F300	1 0 0 0 2	
6.780E-01	6.861E+01	25.04	V013	2 2 2 2 2	
1.976E-01	2.000E+01	65	F300	1 0 0 0 1	

976. $C_6H_{15}N$
N-Ethyl-*sec*-butylamine
sec-Butylethylamine
2-Butanamine, *N*-ethyl-
2-(Ethylamino)butane
RN: 21035-44-9 **MP** (°C)**:**
MW: 101.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.155E-01	8.253E+01	25	D332	0 0 0 0 0	
6.099E-01	6.172E+01	30	D332	0 0 0 0 0	
4.202E-01	4.252E+01	40	D332	0 0 0 0 0	

977. $C_6H_{15}N$
N-Ethyl-*n*-butylamine
Ethylbutylamine
N-Ethylbutan-1-amine
N-Ethylbutylamine
RN: 13360-63-9 **MP** (°C)**:** –78
MW: 101.19 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	1.015E+02	10	D332	0 0 0 0 0	
5.310E-01	5.373E+01	20	D332	0 0 0 0 0	
3.793E-01	3.838E+01	30	D332	0 0 0 0 0	
2.859E-01	2.893E+01	40	D332	0 0 0 0 0	

978. $C_6H_{15}N$
n-Dipropylamine
Dipropylamine
RN: 142-84-7 **MP** (°C)**:** –63
MW: 101.19 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.470E-01	5.536E+01	12.2	H038	1 2 1 1 2	
2.794E-01	2.828E+01	36.1	H038	1 2 1 1 2	
2.335E-01	2.363E+01	44.1	H038	1 2 1 1 2	
1.900E-01	1.922E+01	52.6	H038	1 2 1 1 2	

979. $C_6H_{15}O_2PS_3$
Thiometon
O,*O*-Dimethyl *S*-(2-ethylmercaptoethyl) dithiophosphate
RN: 640-15-3 **MP** (°C)**:**
MW: 246.35 **BP** (°C)**:** 104

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.118E-04	2.000E-01	20	M061	1 0 0 0 2	
8.118E-04	2.000E-01	25	M161	1 0 0 0 2	

980. $C_6H_{15}O_3PS_2$
Thiolo-methylmercaptophos
Thiolo-methyl demeton
RN: **MP** (°C)**:**
MW: 230.29 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-02	3.300E+00	20	M061	1 0 0 0 2	

981. $C_6H_{15}O_3PS_2$
Thiono-methylmercaptophos
Thiono-methyl demeton
RN: **MP** (°C)**:**
MW: 230.29 **BP** (°C)**:** 74

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-03	3.300E-01	20	M061	1 0 0 0 2	

982. $C_6H_{15}O_4P$
Triethyl phosphate
Ethyl phosphate
Phosphoric acid, triethyl ester
TEP
RN: 78-40-0 **MP** (°C)**:** –56.4
MW: 182.16 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.815E+00	5.128E+02	4.50	C022	1 2 0 0 2	
2.745E+00	5.000E+02	25	F300	1 0 0 0 1	
+2.69E+00	+4.90E+02	ns	S460	0 0 0 0 0	

983. $C_6H_{16}FN_2OP$
Mipafox
N,*N*′-Diisopropylphosphorodiamidic fluoride
RN: 371-86-8 **MP** (°C)**:** 65
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.066E-01	7.407E+01	ns	M061	0 0 0 0 0	

984. $C_6H_{16}N_2$
1,6-Hexanediamine
Hexamethylenediamine
RN: 124-09-4 **MP** (°C)**:** 42
MW: 116.21 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E+00	7.115E+02	4.50	C022	1 2 0 0 2	

985. $C_6H_{17}N_3O_{10}S$
Glycine sulfate
Triglycine sulfate
RN: 513-29-1 **MP** (°C)**:**
MW: 323.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.314E-01	1.071E+02	0	M043	1 0 0 0 1	
5.155E-01	1.667E+02	10	M043	1 0 0 0 1	
6.576E-01	2.126E+02	20	M043	1 0 0 0 1	
8.188E-01	2.647E+02	30	M043	1 0 0 0 1	
9.600E-01	3.103E+02	40	M043	1 0 0 0 1	
1.326E+00	4.286E+02	60	M043	1 0 0 0 1	

986. $C_6H_{18}N_4$
Triethylenetetramine
N,*N*′-bis(2-Aminoethyl)-ethylenediamine
1,8-Diamino-3,6-diazaoctane
1,4,7,10-Tetraazadecane
3,6-Diazaoctane-1,8-diamine
Trientine
RN: 112-24-3 **MP** (°C)**:** 12
MW: 146.24 **BP** (°C)**:** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.655E+00	8.269E+02	4.50	C022	1 2 0 0 2	

987. C_6Br_6
Hexabromobenzene
RN: 87-82-1 **MP** (°C)**:** 327
MW: 551.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.558E-11	4.720E-08	10	K440	0 0 0 0 0	
1.994E-10	1.100E-07	25	K440	0 0 0 0 0	
4.207E-10	2.320E-07	35	K440	0 0 0 0 0	

988. $C_6Cl_4O_2$
Chloranil
Tetrachloro-*p*-benzoquinone
2,3,5,6-Tetrachloro-*p*-benzoquinone
2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione
Vulklor
Coversan
RN: 118-75-2 **MP** (°C)**:** 290
MW: 245.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-03	2.500E-01	rt	M161	0 0 0 0 2	

989. $C_6Cl_5NO_2$
Quintozene
Pentachloronitrobenzene
Avical
Eorthcicle
Quintobenzene
RN: 82-68-8 **MP** (°C)**:** >139
MW: 295.34 **BP** (°C)**:** 328

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.430E-04	20	E308	1 2 2 1 1	
1.862E-06	5.500E-04	22	K137	1 1 2 1 0	
1.490E-06	4.400E-04	22.5	G301	0 0 0 0 0	

990. C_6Cl_6
Hexachlorobenzene
Benzene hexachloride
HCB
Hexa-chlorobenzene
RN: 118-74-1 **MP** (°C)**:** 228
MW: 284.78 **BP** (°C)**:** 324.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.585E-05	20	B179	0 0 0 0 0	
1.721E-08	4.900E-06	20	C113	1 0 1 1 1	
2.598E-08	7.400E-06	20	H300	1 1 2 2 1	
1.896E-08	5.400E-06	20	H300	1 1 2 2 1	
2.042E-08	5.815E-06	20	K337	1 0 0 0 2	
1.380E-08	3.931E-06	22	K305	1 0 1 1 2	
1.756E-08	5.000E-06	22.5	G301	0 0 0 0 0	
1.700E-08	4.841E-06	25	B317	0 0 0 0 0	
1.650E-08	4.699E-06	25	M342	1 0 1 1 2	
2.107E-08	6.000E-06	26.70	L095	2 2 1 1 2	
<3.51E-06	<1.00E-03	30	M311	1 1 2 2 0	
7.023E-08	2.000E-05	ns	L072	0 0 0 0 1	
2.107E-08	6.000E-06	ns	L311	0 0 0 0 1	
1.650E-07	4.699E-05	ns	M308	0 0 1 1 2	
2.458E-05	7.000E-03	rt	H053	0 2 2 2 0	γ isomer

991. C_6F_6
Hexafluorobenzene
Perfluorobenzene
RN: 392-56-3 **MP** (°C)**:** 3.9 C
MW: 186.06 **BP** (°C)**:** 81 C at 743 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-03	7.788E-01	8.30	F418	0 0 0 0 0	
3.598E-03	6.694E-01	18.20	F418	0 0 0 0 0	
3.315E-03	6.167E-01	27.81	F418	0 0 0 0 0	
3.198E-03	5.950E-01	37.66	F418	0 0 0 0 0	
3.148E-03	5.857E-01	47.35	F418	0 0 0 0 0	
3.209E-03	5.971E-01	56.61	F418	0 0 0 0 0	
3.420E-03	6.363E-01	66.60	F418	0 0 0 0 0	

992. $C_7H_3Br_2NO$
Bromoxynil
3,5-Dibromo-4-hydroxybenzonitrile
4-Cyano-2,6-dibromophenol
RN: 1689-84-5 **MP** (°C)**:** 190
MW: 276.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.694E-04	1.300E-01	25	M161	1 0 0 0 2	
4.694E-04	1.300E-01	ns	M061	0 0 0 0 2	

993. $C_7H_3Br_3O_2$
2,4,6-Tribromobenzoic acid
2,4,6-Tribrom-benzoesaeure
RN: 633-12-5 **MP** (°C)**:**
MW: 358.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.754E-03	3.500E+00	15	F300	1 0 0 0 1	
1.533E-02	5.500E+00	100	F300	1 0 0 0 1	

994. $C_7H_3Cl_2N$
Dichlobenil
2,6-Dichlorobenzonitrile
Benzonitrile, 2,6-dichloro-
RN: 1194-65-6 **MP** (°C)**:** 145
MW: 172.01 **BP** (°C)**:** 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.046E-04	1.800E-02	20	B185	0 0 0 0 0	
1.046E-04	1.800E-02	20	B200	1 0 0 1 1	
1.046E-04	1.800E-02	20	G319	0 0 0 0 0	
1.046E-04	1.800E-02	20	M161	1 0 0 0 1	
1.163E-04	2.000E-02	25	B185	0 0 0 0 0	
5.813E-05	1.000E-02	25	M061	1 0 0 0 1	
1.046E-04	1.800E-02	ns	V303	0 0 0 0 1	

995. $C_7H_3Cl_3O_2$
2,3,6-Trichlorobenzoic acid
2,3,6-TBA
RN: 50-31-7 **MP** (°C)**:** 125
MW: 225.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.726E-02	8.400E+00	20	B200	1 0 0 0 1	
3.415E-02	7.700E+00	22	M161	1 0 0 0 1	

996. $C_7H_3Cl_5O$
Pentachlorbenzyl alcohol
Blastin
PCBA
RN: 16022-69-8 **MP** (°C)**:**
MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.134E-07	2.000E-04	25	M061	0 0 0 0 0	

997. $C_7H_3I_2NO$
Ioxynil
4-Cyano-2,6-diiodophenol
4-Hydroxy-3,5-diiodobenzonitrile
RN: 1689-83-4 **MP** (°C)**:** 212
MW: 370.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.348E-04	5.000E-02	20	F311	1 2 2 2 1	
3.505E-04	1.300E-01	25	B200	1 0 0 0 2	
1.348E-04	5.000E-02	25	M161	1 0 0 0 1	

998. $C_7H_3N_3O_8$
2,4,6-Trinitrobenzoic acid
2,4,6-Trinitrobenzoesaeure
Acide 2,4,6-trinitrobenzoique
RN: 129-66-8 **MP** (°C)**:** 228.7
MW: 257.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-02	2.010E+01	23	F300	1 0 0 0 2	
7.824E-02	2.012E+01	23.5	D067	1 2 0 0 2	
1.560E-01	4.012E+01	50	D067	1 2 0 0 2	
1.560E-01	4.010E+01	50	F300	1 0 0 0 2	

999. C_7H_4BrN
4-Bromobenzonitrile
p-Bromobenzonitrile
4-Bromobenzoic acid nitrile
RN: 623-00-7 **MP** (°C)**:** 111 C
MW: 182.03 **BP** (°C)**:** 236 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.635E-04	1.572E-01	22	J420	0 0 0 0 0	pH 6.5

1000. $C_7H_4BrNO_4$
3-Bromo-2-nitrobenzoic acid
Benzoic acid, 3-bromo-2-nitro-
RN: 116529-61-4 **MP** (°C)**:**
MW: 246.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.012E-02	7.410E+00	25	H089	1 2 0 0 2	
1.341E-03	3.300E-01	25	H089	1 2 0 0 1	

1001. C_7H_4BrNS
4-Bromophenyl isothiocyanate
1-Bromo-4-isothiocyanato-benzene
RN: 1985-12-2 **MP** (°C)**:** 60.5
MW: 214.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	1.156E-02	25	D019	1 1 1 1 1	

1002. C_7H_4BrNS
3-Bromophenyl isothiocyanate
1-Bromo-3-isothiocyanato-benzene
RN: 2131-59-1 **MP** (°C)**:**
MW: 214.09 **BP** (°C)**:** 256.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	2.441E-02	25	D019	1 1 1 1 2	
8.200E-05	1.756E-02	25	K032	2 2 0 1 1	

1003. $C_7H_4ClNO_4$
3-Chloro-2-nitrobenzoic acid
2-Nitro-3-chlorobenzoic acid
RN: 4771-47-5 **MP** (°C)**:**
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.332E-03	4.700E-01	25	H089	1 2 0 0 1	

1004. $C_7H_4ClNO_4$
4-Chloro-3-nitrobenzoic acid
3-Nitro-4-chlorobenzoic acid
RN: 96-99-1 **MP** (°C)**:** 181
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	3.427E-01	ns	C014	0 0 0 1 1	

1005. $C_7H_4ClNO_4$
5-Chloro-2-nitrobenzoic acid
2-Nitro-5-chlorobenzoic acid
RN: 2516-95-2 **MP** (°C)**:**
MW: 201.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-02	9.670E+00	25	H089	1 2 0 0 2	

1006. C_7H_4ClNS
3-Chlorophenyl isothiocyanate
1-Chloro-3-isothiocyanato-benzene
RN: 2392-68-9 **MP** (°C)**:**
MW: 169.63 **BP** (°C)**:** 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.393E-02	25	D019	1 1 1 1 0	
1.120E-04	1.900E-02	25	K032	2 2 0 1 2	

1007. $C_7H_4Cl_2O_2$
3,5-Dichlorobenzoic acid
Benzoic acid, 3,5-dichloro-
RN: 51-36-5 **MP** (°C)**:** 186
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-04	1.471E-01	ns	C014	0 0 0 1 1	

1008. $C_7H_4Cl_2O_2$
2,6-Dichlorobenzoic acid
2,6-Dichlor-benzoesaeure
RN: 50-30-6 **MP** (°C)**:**
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.414E+01	ns	C014	0 0 0 1 1	

1009. $C_7H_4Cl_2O_2$
2,4-Dichlorobenzoic acid
2,4-Dichlor-benzoesaeure
RN: 50-84-0 **MP** (°C)**:**
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.775E-01	ns	C014	0 2 0 1 1	

1010. $C_7H_4Cl_2O_2$
3,4-Dichlorobenzoic acid
Benzoic acid, 3,4-dichloro-
RN: 51-44-5 **MP** (°C)**:** 208
MW: 191.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	6.112E-02	ns	C014	0 0 0 1 1	

1011. $C_7H_4Cl_3NO_3$
Triclopyr
Garlon
(3,5,6-Trichloro-2-pyridinyl)oxyacetic acid
Crossbow turflon
RN: 55335-06-3 **MP** (°C)**:** 149
MW: 256.47 **BP** (°C)**:** 290

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.300E-01	ns	K138	0 0 0 0 1	

1012. $C_7H_4Cl_4O$
2,4,5,6-Tetrachloro-3-methyl-phenol
m-Cresol, 2,4,5,6-tetrachloro-
Phenol, 2,3,4,6-tetrachloro-5-methyl-
RN: 10460-33-0 **MP** (°C)**:**
MW: 245.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.148E-03	25	B316	0 0 0 0 0	

1013. $C_7H_4Cl_4O$
2,3,4,5-Tetrachloroanisole
Benzene, 1,2,3,4-tetrachloro-5-methoxy-
Anisole, 2,3,4,5-tetrachloro-
RN: 938-86-3 **MP** (°C)**:** 88
MW: 245.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.490E-06	1.350E-03	25	L348	1 2 2 1 2	

1014. C_7H_4INS
4-Iodophenyl isothiocyanate
4-Iodophenylisothiocyanate
RN: 2059-76-9 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.350E-02	25	D019	1 1 1 1 1	

1015. C_7H_4INS

3-Iodophenyl isothiocyanate
m-Iodophenyl isothiocyanate
RN: 3125-73-3 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.483E-03	25	K032	2 2 0 1 0	

1016. $C_7H_4I_2O_3$

3,5-Diiodosalicylic acid
2-Hydroxy-3,5-diiod-benzoesaeure
RN: 133-91-5 **MP** (°C)**:** 235.5
MW: 389.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.274E-04	1.666E-01	10	C072	1 2 1 1 2	
1.795E-03	7.000E-01	15	F300	1 0 0 0 1	
4.931E-04	1.923E-01	25	C072	1 2 1 1 2	
3.847E-03	1.500E+00	h	F300	1 0 0 0 1	

1017. $C_7H_4N_2O_2S$

3-Nitrophenyl isothiocyanate
m-Nitrophenylisothiocyanate
RN: 3529-82-6 **MP** (°C)**:**
MW: 180.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-04	5.045E-02	25	K032	2 2 0 1 2	

1018. $C_7H_4N_2O_6$

2,4-Dinitrobenzoic acid
2,4-Dinitrobenzoesaeure
RN: 610-30-0 **MP** (°C)**:**
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.580E-02	1.820E+01	25	F300	1 0 0 0 2	
4.900E-02	1.039E+01	ns	C014	0 0 0 1 1	

1019. $C_7H_4N_2O_6$
2,6-Dinitrobenzoic acid
2,6-Dinitrobenzoesaeure
RN: 603-12-3 **MP** (°C)**:**
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	1.612E+01	ns	C014	0 2 0 1 1	

1020. $C_7H_4N_2O_6$
3,4-Dinitrobenzoic acid
3,4-Dinitrobenzoesaeure
RN: 528-45-0 **MP** (°C)**:** 166
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-02	6.700E+00	25	F300	1 0 0 0 1	

1021. $C_7H_4N_2O_6$
3,5-Dinitrobenzoic acid
3,5-Dinitrobenzoesaeure
RN: 99-34-3 **MP** (°C)**:** 205
MW: 212.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.347E+00	25	K040	1 0 2 1 2	
2.923E-03	6.200E-01	25	P037	2 0 1 1 1	

1022. $C_7H_4N_4O_9$
2,3,5,6-Tetranitroanisol
RN: **MP** (°C)**:**
MW: 288.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.941E-04	2.000E-01	50	F300	1 0 0 0 0	
4.165E-03	1.200E+00	100	F300	1 0 0 0 1	

1023. $C_7H_4O_6$
Chelidonic acid
Chelidonsaeure
RN: 99-32-1 **MP** (°C)**:**
MW: 184.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.767E-02	1.430E+01	25	F300	1 0 0 0 2	
2.064E-01	3.800E+01	100	F300	1 0 0 0 1	

1024. $C_7H_4O_7$
Meconic acid
Mekonsaeure
RN: 497-59-6 **MP** (°C)**:**
MW: 200.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.198E-02	8.400E+00	25	F300	1 0 0 0 1	
1.034E+00	2.070E+02	100	F300	1 0 0 0 2	

1025. $C_7H_5BrO_2$
p-Bromobenzoic acid
4-Bromobenzoic acid
RN: 586-76-5 **MP** (°C)**:** 252.0
MW: 201.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-04	5.600E-02	22.5	G301	0 0 0 0 0	
2.985E-04	6.000E-02	ns	B150	0 0 2 2 1	
2.885E-04	5.800E-02	ns	B150	0 0 2 2 1	
2.800E-04	5.629E-02	ns	C014	0 0 0 1 1	

1026. $C_7H_5BrO_2$
m-Bromobenzoic acid
3-Bromobenzoic acid
RN: 585-76-2 **MP** (°C)**:** 155
MW: 201.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.021E-01	ns	C014	0 0 0 1 1	

1027. $C_7H_5ClN_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(chloroacetyl)-1,5-dihydro-
RN: 96448-62-3 **MP** (°C)**:**
MW: 212.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.174E-04	1.100E-01	22	B428	1 2 1 2 1	

1028. $C_7H_5ClO_2$

meta-Chlorobenzoic acid
3-Chlorobenzoic acid
m-Chlorobenzoic acid
3-Chlor-benzoesaeure

RN: 535-80-8 **MP** (°C)**:** 154
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-04	4.000E-02	0	F300	1 0 0 0 0	
4.080E-03	6.388E-01	24.99	B391	0 0 0 0 0	
2.555E-03	4.000E-01	25	F300	1 0 0 0 0	
2.543E-03	3.982E-01	25	T066	1 0 0 0 2	
2.555E-03	4.000E-01	37	M360	1 2 1 1 2	
2.460E-03	3.852E-01	ns	O004	0 2 1 1 2	

1029. $C_7H_5ClO_2$

p-Chlorobenzoic acid
4-Chlorobenzoic acid
Chloradracylic
4-Chlor-benzoesaeure

RN: 74-11-3 **MP** (°C)**:** 235
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-04	9.000E-02	22.5	G301	0 0 0 0 0	
8.000E-04	1.253E-01	24.99	B391	0 0 0 0 0	
7.026E-04	1.100E-01	25	C410	2 0 2 2 1	
4.918E-04	7.700E-02	25	F300	1 0 0 0 1	
4.639E-04	7.263E-02	25	T066	1 0 0 0 2	
7.026E-04	1.100E-01	37	M360	1 2 1 1 2	
4.918E-04	7.700E-02	ns	B150	0 0 2 2 1	
4.350E-04	6.811E-02	ns	O004	0 2 1 1 2	

1030. $C_7H_5ClO_2$

o-Chlorobenzoic acid
2-Chlor-benzoesaeure
2-Chlorobenzoic acid

RN: 118-91-2 **MP** (°C)**:** 142
MW: 156.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.288E+00	24.99	B391	0 0 0 0 0	
1.916E-02	3.000E+00	25	C410	2 0 2 2 1	
1.341E-02	2.100E+00	25	F300	1 0 0 0 1	
8.686E-03	1.360E+00	25	P037	2 0 1 1 2	
1.865E-02	2.920E+00	37	M360	1 2 1 1 2	
2.574E-01	4.030E+01	100	F300	1 0 0 0 2	
1.330E-02	2.082E+00	ns	C014	0 0 0 1 2	
1.362E-02	2.132E+00	ns	O004	0 2 1 1 2	

1031. $C_7H_5Cl_2NO$
2,6-Dichlorobenzamide
Dichlorobenzamide
BAM
RN: 2008-58-4 **MP** (°C)**:** 198
MW: 190.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E-02	2.700E+00	22.5	G301	0 0 0 0 0	

1032. $C_7H_5Cl_2NO_2$
Chloramben
3-Amino-2,5-dichlorobenzoic acid
RN: 133-90-4 **MP** (°C)**:** 201
MW: 206.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-03	7.000E-01	25	B200	1 0 0 0 2	
3.398E-03	7.000E-01	25	M161	1 0 0 0 2	
3.398E-03	7.000E-01	ns	B185	0 0 0 0 0	

1033. $C_7H_5Cl_2NS$
2,6-Dichlorothiobenzamide
Prefix
Chlorthiamid
RN: 1918-13-4 **MP** (°C)**:** 151.5
MW: 206.09 **BP** (°C)**:** 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.561E-03	9.400E-01	20	M061	1 0 0 0 2	
4.610E-03	9.500E-01	21	M161	1 0 0 0 2	

1034. $C_7H_5Cl_3O$
2,3,4-Trichloroanisole
1,2,3-Trichloro-4-methoxy-benzene
RN: 54135-80-7 **MP** (°C)**:** 70
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.107E-05	1.080E-02	25	L348	1 2 2 1 2	

1035. $C_7H_5Cl_3O$

2,4,6-Trichloro-3-methylphenol
m-Cresol, 2,4,6-trichloro-
2,4,6-Trichloro-*m*-cresol
RN: 551-76-8 **MP** (°C)**:**
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.121E-01	25	B316	0 0 0 0 0	

1036. $C_7H_5Cl_3O$

2,4,6-Trichloroanisole
1-Methoxy-2,4,6-trichlorobenzene
Methyl 2,4,6-trichlorophenyl ether
Tyrene
RN: 87-40-1 **MP** (°C)**:** 61
MW: 211.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-05	1.320E-02	25	L348	1 2 2 1 2	

1037. $C_7H_5FO_2$

m-Fluorobenzoic acid
3-Fluor-benzoesaeure
3-Fluorobenzoic acid
RN: 455-38-9 **MP** (°C)**:** 123
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.071E-02	1.500E+00	25	F300	1 0 0 0 1	

1038. $C_7H_5FO_2$

o-Fluorobenzoic acid
2-Fluorobenzoic acid
RN: 445-29-4 **MP** (°C)**:** 123
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-02	7.200E+00	25	F300	1 0 0 0 1	
5.129E-02	7.186E+00	ns	R427	0 0 0 0 0	

1039. $C_7H_5FO_2$
p-Fluorobenzoic acid
4-Fluor-benzoesaeure
4-Fluorobenzoic acid
RN: 456-22-4 **MP** (°C)**:** 182.6
MW: 140.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.564E-03	1.200E+00	25	F300	1 0 0 0 1	

1040. $C_7H_5F_3N_2O_4S$
3-Trifluoromethyl-4-nitrobenzenesulfonamide
4-Nitro-3-(trifluoromethyl)benzenesulfonamide
RN: 21988-05-6 **MP** (°C)**:**
MW: 270.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-04	1.756E-01	15	K024	1 2 1 1 2	

1041. $C_7H_5IO_2$
p-Iodobenzoic acid
4-Iodobenzoic acid
RN: 619-58-9 **MP** (°C)**:**
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	2.778E-02	15	D008	1 0 1 1 2	intrinsic

1042. $C_7H_5IO_2$
o-Iodobenzoic acid
2-Iodobenzoic acid
RN: 88-67-5 **MP** (°C)**:** 162
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.860E-03	4.613E-01	15	D008	1 0 1 1 2	0.002N HCl

1043. $C_7H_5IO_2$
m-Iodobenzoic acid
3-Iodobenzoic acid
RN: 618-51-9 **MP** (°C)**:** 187
MW: 248.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-04	1.334E-01	15	D008	1 0 1 1 2	0.002N HCl

1044. $C_7H_5I_2NO_3$
3,5-Diiodo-4-pyridone-*N*-acetic acid
3,5-Diiod-pyridon-(4)-*N*-essigsaeure
3,5-Diiodo-4-pyridone-1-acetic acid
Diodon
1,4-Dihydro-3,5-diiodo-4-oxopyridine-1-acetic acid
RN: 101-29-1 **MP** (°C)**:** 244
MW: 404.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.883E-03	2.787E+00	ns	H055	0 0 0 0 0	

1045. C_7H_5N
Benzonitrile
Benzonitril
Benzenenitrile
Benzoic acid nitrile
Phenyl cyanide
Cyanobenzene
RN: 100-47-0 **MP** (°C)**:** –13
MW: 103.12 **BP** (°C)**:** 190.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.839E-02	1.896E+00	24.0	P321	0 0 0 0 0	
4.200E-02	4.331E+00	25	M327	1 0 0 1 2	
3.671E-02	3.786E+00	35.5	P321	0 0 0 0 0	
5.400E-02	5.569E+00	50.0	P321	0 0 0 0 0	
4.056E-02	4.182E+00	57.0	P321	0 0 0 0 0	
5.496E-02	5.668E+00	62.5	P321	0 0 0 0 0	
8.268E-02	8.527E+00	85.0	P321	0 0 0 0 0	
8.459E-02	8.723E+00	90.5	P321	0 0 0 0 0	
9.981E-02	1.029E+01	95.5	P321	0 0 0 0 0	
9.697E-02	1.000E+01	100	F300	1 0 0 0 0	
1.065E-01	1.098E+01	101.0	P321	0 0 0 0 0	
1.339E-01	1.381E+01	116.0	P321	0 0 0 0 0	
1.920E-01	1.980E+01	127.5	P321	0 0 0 0 0	
2.171E-01	2.239E+01	142.0	P321	0 0 0 0 0	
2.888E-01	2.979E+01	148.0	P321	0 0 0 0 0	
2.834E-01	2.922E+01	149.0	P321	0 0 0 0 0	
3.873E-01	3.994E+01	160.5	P321	0 0 0 0 0	
5.747E-01	5.927E+01	164.5	P321	0 0 0 0 0	
1.373E+00	1.416E+02	201.0	P321	0 0 0 0 0	
2.937E+00	3.029E+02	211.0	P321	0 0 0 0 0	
9.696E-04	9.999E-02	ns	L055	0 0 0 0 1	

1046. C_7H_5NOS

4-Hydroxyphenyl isothiocyanate
4-Hydroxyphenylisothiocyanate
RN: 2131-60-4 **MP** (°C)**:**
MW: 151.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.150E-03	3.251E-01	25	D019	1 1 1 1 2	

1047. C_7H_5NOS

3-Hydroxyphenyl isothiocyanate
m-Hydroxyphenyl isothiocyanate
RN: 3125-63-1 **MP** (°C)**:**
MW: 151.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.542E+00	25	K032	2 2 0 1 2	
1.023E-02	1.547E+00	ns	R427	0 0 0 0 0	

1048. $C_7H_5NO_3$

m-Nitrobenzaldehyde
3-Nitrobenzaldehyde
3-Nitro-benzaldehyd
RN: 99-61-6 **MP** (°C)**:** 58
MW: 151.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.617E-05	1.000E-02	25	F300	1 0 0 0 1	
3.309E+00	5.000E+02	58.0	S118	1 2 0 1 0	
6.292E-02	9.509E+00	75.1	S118	1 2 0 1 1	
3.272E+00	4.945E+02	85.2	S118	1 2 0 1 2	
1.266E-01	1.913E+01	111.9	S118	1 2 0 1 2	
1.934E-01	2.922E+01	136.4	S118	1 2 0 1 2	
3.103E-01	4.689E+01	157.3	S118	1 2 0 1 2	
6.293E-01	9.510E+01	181.0	S118	1 2 0 1 2	
8.142E-01	1.230E+02	191.4	S118	1 2 0 1 2	
1.253E+00	1.893E+02	205.4	S118	1 2 0 1 2	
1.878E+00	2.838E+02	211.8	S118	1 2 0 1 2	

1049. $C_7H_5NO_3$
o-Nitrobenzaldehyde
2-Nitrobenzaldehyde
2-Nitro-benzaldehyd
RN: 552-89-6 **MP** (°C)**:** 44
MW: 151.12 **BP** (°C)**:** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-04	2.000E-02	25	F300	1 0 0 0 1	
4.600E-02	6.951E+00	66.9	S118	1 2 0 1 1	
9.972E-02	1.507E+01	103.1	S118	1 2 0 1 1	
3.001E-01	4.535E+01	166.0	S118	1 2 0 1 1	

1050. $C_7H_5NO_3$
p-Nitrobenzaldehyde
4-Nitrobenzaldehyde
RN: 555-16-8 **MP** (°C)**:** 106.5
MW: 151.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.871E-01	2.828E+01	132.4	S118	1 2 0 1 2	
5.341E-01	8.071E+01	176.5	S118	1 2 0 1 2	
1.133E+00	1.713E+02	205.4	S118	1 2 0 1 2	
1.814E+00	2.742E+02	215.5	S118	1 2 0 1 2	

1051. $C_7H_5NO_3S$
Saccharin
1,1-Dioxide-1,2-benzisothiazol-3-(2H)-one
3-Benzisothiazolinone 1,1-dioxide
1,2-Benzisothiazol-3(2H)-one-1,1-dioxide
Kandiset
Glucid
RN: 81-07-2 **MP** (°C)**:** 228.8
MW: 183.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-02	4.300E+00	25	F300	1 0 0 0 1	
1.880E-01	3.444E+01	30	M015	1 0 2 1 0	EFG

1052. $C_7H_5NO_4$
Quinolinic acid
2,3-Pyridinedicarboxylic acid
Pyridine-2,3-dicarboxylic acid
Pyridine-2,3-dicarboxylate
RN: 89-00-9 **MP** (°C)**:** 190
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	5.500E+00	7	F300	1 0 0 0 1	
6.600E-02	1.103E+01	25	C104	2 2 1 1 2	
6.400E-02	1.070E+01	25	C104	2 2 1 1 2	

1053. $C_7H_5NO_4$
p-Nitrobenzoic acid
4-Nitrobenzoic acid
RN: 62-23-7 **MP** (°C)**:** 242.4
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-03	2.000E-01	15	F300	1 0 0 0 2	
2.525E-03	4.220E-01	24.99	B391	0 0 0 0 0	
1.660E-03	2.774E-01	25	H071	2 2 2 1 2	
3.471E-03	5.800E-01	37	B171	2 0 1 1 2	

1054. $C_7H_5NO_4$
o-Nitrobenzoic acid
2-Nitrobenzoic acid
RN: 552-16-9 **MP** (°C)**:** 147.5
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-02	6.551E+00	18	D058	1 0 1 1 2	
3.340E-02	5.582E+00	24.99	B391	0 0 0 0 0	
4.325E-02	7.228E+00	25	D058	1 0 1 1 2	
4.488E-02	7.500E+00	25	F300	1 0 0 0 1	
4.350E-02	7.270E+00	25	H071	2 2 2 1 2	
4.700E-02	7.855E+00	25	K040	1 0 2 1 2	
4.360E-02	7.287E+00	25	K053	2 2 2 2 2	
4.430E-02	7.404E+00	25	L050	2 0 1 2 2	
4.415E-02	7.378E+00	25	R016	0 0 0 0 0	
4.700E-02	7.855E+00	26.4	P043	2 0 1 1 2	

1055. $C_7H_5NO_4$
m-Nitrobenzoic acid
3-Nitrobenzoic acid
RN: 121-92-6 **MP** (°C)**:** 142.0
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.436E-02	2.400E+00	15	F300	1 0 0 0 1	
1.530E-02	2.557E+00	24.99	B391	0 0 0 0 0	
2.121E-02	3.545E+00	25	C076	0 0 0 0 0	
2.140E-02	3.576E+00	25	K040	1 0 2 1 2	
1.227E-02	2.050E+00	25	P037	2 0 1 1 2	
6.582E-02	1.100E+01	37	B171	2 0 1 1 2	
2.334E-02	3.900E+00	ns	B361	0 0 0 0 0	

1056. $C_7H_5NO_4$
Isocinchomeronic acid
2,5-Pyridinedicarboxylic acid
Pyridine-2,5-dicarboxylic acid
RN: 100-26-5 **MP** (°C)**:** 254
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.237E+00	25	C104	2 2 1 1 2	
7.100E-03	1.187E+00	25	C104	2 2 1 1 2	

1057. $C_7H_5NO_4$
Cinchomeronic acid
3,4-Pyridinedicarboxylic acid
RN: 490-11-9 **MP** (°C)**:** 256
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	2.340E+00	25	C104	2 2 1 1 2	
1.380E-02	2.306E+00	25	C104	2 2 1 1 2	

1058. $C_7H_5NO_4$
3,5-Pyridinedicarboxylic acid
Dinicotinic acid
RN: 499-81-0 **MP** (°C)**:**
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.070E+00	25	C104	2 2 1 1 2	

1059. $C_7H_5NO_4$
4-Formyl-2-NO2-phenol
RN: **MP** (°C)**:**
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.122E-03	1.875E-01	ns	R424	0 0 0 0 0	

1060. $C_7H_5NO_4$
Lutidinic acid
2,4-Pyridinedicarboxylic acid
RN: 499-80-9 **MP** (°C)**:** 248
MW: 167.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-02	2.490E+00	25	C104	2 2 1 1 2	
1.480E-02	2.473E+00	25	C104	2 2 1 1 2	

1061. $C_7H_5NO_5$
3-Nitrosalicylic acid
3-Nitro-salicylsaeure
RN: 85-38-1 **MP** (°C)**:** 128
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.099E-03	1.300E+00	16	F300	1 0 0 0 1	

1062. $C_7H_5NO_5$
5-Nitrosalicylic acid
5-Nitrosalicylsaeure
RN: 96-97-9 **MP** (°C)**:** 229–230
MW: 183.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-02	2.000E+00	45	F300	1 0 0 0 0	

1063. C_7H_5NS
Benzothiazole
Benzthiazol
RN: 95-16-9 **MP** (°C)**:** 2
MW: 135.19 **BP** (°C)**:** 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	4.275E+00	ns	S460	0 0 0 0 0	

1064. C_7H_5NS
Phenyl isothiocyanate
Isothiocyanatobenzene
Phenyl mustard oil
PITC
RN: 103-72-0 **MP** (°C)**:** –21.0
MW: 135.19 **BP** (°C)**:** 221.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-04	8.990E-02	25	D019	1 1 1 1 2	

1065. $C_7H_5N_3O_6$
2,4,6-Trinitrotoluene
2,4,6-Tronitrotoluol
RN: 118-96-7 **MP** (°C)**:** 80.1
MW: 227.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-04	1.100E-01	.3	D065	1 2 2 1 2	
4.842E-04	1.100E-01	.3	T020	1 2 2 2 2	
4.843E-04	1.100E-01	.30	F300	1 0 0 0 1	
4.975E-04	1.130E-01	5.9	D065	1 2 2 1 2	
4.974E-04	1.130E-01	5.9	T020	1 2 2 2 2	
5.283E-04	1.200E-01	20	D065	1 2 2 1 2	
5.283E-04	1.200E-01	20.0	T020	1 2 2 2 2	
8.937E-04	2.030E-01	33.1	D065	1 2 2 1 2	
8.936E-04	2.030E-01	33.1	T020	1 2 2 2 2	
1.497E-03	3.400E-01	44.2	D065	1 2 2 1 2	
1.496E-03	3.399E-01	44.2	T020	1 2 2 2 2	
1.629E-03	3.700E-01	45	D065	1 2 2 1 2	
1.628E-03	3.699E-01	45.0	T020	1 2 2 2 2	
2.351E-03	5.340E-01	53	D065	1 2 2 1 2	
2.350E-03	5.337E-01	53.0	T020	1 2 2 2 2	
2.703E-03	6.140E-01	57.1	D065	1 2 2 1 2	
2.702E-03	6.136E-01	57.1	T020	1 2 2 2 2	
4.240E-03	9.630E-01	73.2	D065	1 2 2 1 2	
4.236E-03	9.621E-01	73.2	T020	1 2 2 2 2	
6.054E-03	1.375E+00	94.4	D065	1 2 2 1 2	
6.045E-03	1.373E+00	94.4	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.5	D065	1 2 2 1 2	
6.449E-03	1.465E+00	99.5	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.50	F300	1 0 0 0 2	
6.026E-04	1.369E-01	ns	R427	0 0 0 0 0	

1066. $C_7H_5N_3O_7$
2,4,6-Trinitro-*m*-cresol
2,4,6-Trinitro-*m*-kresol
RN: 3238-38-8 **MP** (°C)**:**
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.226E-03	2.000E+00	15	F300	1 0 0 0 0	

1067. $C_7H_5N_3O_7$
Methyl picric acid
2,4,6-Trinitro-3-methylphenol
3-Methyl-2,4,6-trinitrophenol
2,4,6-Trinitro-*m*-cresol
RN: 602-99-3 **MP** (°C)**:**
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	2.431E+00	25	K053	2 2 2 2 2	

1068. $C_7H_5N_3O_7$
2,4,6-Trinitroanisole
2-Methoxy-1,3,5-trinitro-benzene
Methyl picrate
RN: 606-35-9 **MP** (°C)**:** 69
MW: 243.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.224E-04	2.000E-01	15	D079	1 2 0 0 1	
5.627E-03	1.368E+00	50	D079	1 2 0 0 2	
1.594E-02	3.875E+00	100	D079	1 2 0 0 2	

1069. $C_7H_5N_5O_8$
Nitramine
Tetryl
N-Methyl-*N*,2,4,5-tetranitroaniline
RN: 479-45-8 **MP** (°C)**:** 131
MW: 287.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.776E-04	5.100E-02	.5	T015	1 2 0 1 1	
1.776E-04	5.100E-02	.50	D066	1 2 2 1 2	
1.741E-04	5.000E-02	.50	F300	1 0 0 0 0	
2.403E-04	6.900E-02	9.6	D066	1 2 2 1 2	
2.403E-04	6.900E-02	9.6	T015	1 2 0 1 1	
2.473E-04	7.100E-02	14.8	D066	1 2 2 1 1	

(*continued*)

1069. $C_7H_5N_5O_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-04	7.099E-02	14.8	T015	1 2 0 1 1	
2.577E-04	7.400E-02	20.5	D066	1 2 2 1 1	
2.577E-04	7.399E-02	20.5	T015	1 2 0 1 1	
2.925E-04	8.400E-02	30	D066	1 2 2 1 1	
2.925E-04	8.399E-02	30.0	T015	1 2 0 1 1	
3.274E-04	9.400E-02	35	D066	1 2 2 1 1	
3.273E-04	9.399E-02	35.0	T015	1 2 0 1 1	
3.726E-04	1.070E-01	40	D066	1 2 2 1 2	
3.726E-04	1.070E-01	40.0	T015	1 2 0 1 2	
4.701E-04	1.350E-01	45	D066	1 2 2 1 2	
4.701E-04	1.350E-01	45.0	T015	1 2 0 1 2	
6.965E-04	2.000E-01	50	D066	1 2 2 1 2	
6.964E-04	2.000E-01	50.0	T015	1 2 0 1 2	
1.219E-03	3.500E-01	60	D066	0 0 0 0 0	
1.218E-03	3.499E-01	60.05	T015	1 2 0 1 2	
1.543E-03	4.430E-01	65	D065	1 2 2 1 2	
1.542E-03	4.428E-01	65.05	T015	1 2 0 1 2	
1.849E-03	5.310E-01	69.5	D065	1 2 2 1 2	
1.848E-03	5.307E-01	69.5	T015	1 2 0 1 2	
3.315E-03	9.520E-01	84.2	D065	1 2 2 1 2	
3.312E-03	9.511E-01	84.2	T015	1 2 0 1 2	
5.638E-03	1.619E+00	96.7	D065	1 2 2 1 2	
5.629E-03	1.616E+00	96.7	T015	1 2 0 1 2	
6.112E-03	1.755E+00	98.5	D065	1 2 2 1 2	
6.101E-03	1.752E+00	98.55	T015	1 2 0 1 2	
6.129E-03	1.760E+00	99	F300	1 0 0 0 2	

1070. C_7H_6ClF
2-Fluorobenzyl chloride
o-Fluorobenzyl chloride
RN: 345-35-7 **MP** (°C)**:**
MW: 144.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.880E-03	4.164E-01	25	M342	1 0 1 1 2	
2.877E-03	4.160E-01	ns	S460	0 0 0 0 0	

1071. C_7H_6ClF
3-Fluorobenzyl chloride
m-Fluorobenzyl chloride
RN: 456-42-8 **MP** (°C)**:**
MW: 144.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-03	4.135E-01	25	M342	1 0 1 1 2	
2.858E-03	4.131E-01	ns	S460	0 0 0 0 0	

1072. C_7H_6ClF
4-Fluorobenzyl chloride
1-(Chloromethyl)-4-fluoro-benzene
α-Chloro-*p*-fluorotoluene
RN: 352-11-4 **MP** (°C)**:** –18
MW: 144.58 **BP** (°C)**:** 181.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.884E-03	4.170E-01	ns	S460	0 0 0 0 0	

1073. $C_7H_6ClN_3O_4S_2$
Chlorothiazide
Diuresal
RN: 58-94-6 **MP** (°C)**:** 342
MW: 295.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-04	2.827E-01	25	A076	1 0 1 1 2	
9.000E-04	2.662E-01	30	A089	2 0 1 1 0	EFG
9.000E-04	2.662E-01	30	A093	2 0 1 1 0	EFG
6.763E-04	2.000E-01	ns	C114	0 0 0 0 0	
7.439E-04	2.200E-01	rt	A095	0 0 2 2 1	
9.806E-04	2.900E-01	rt	B181	0 0 1 1 2	

1074. $C_7H_6ClN_4O_5S_2$
4-Nitroso-hydrochlorothiazide
RN: **MP** (°C)**:** 155–156
MW: 325.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.368E-04	2.400E-01	25	G051	1 0 1 1 0	

1075. $C_7H_6Cl_2N_2O$
Chlorambenamide
3,5-Dichloroanthranilamide
Benzamide, 2-amino-3,5-dichloro-
RN: 36765-01-2 **MP** (°C)**:** 162.5
MW: 205.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.291E-03	1.700E+00	rt	M161	0 0 0 0 1	

1076. $C_7H_6Cl_2O$
2,6-Dichloroanisole
Benzene, 1,3-dichloro-2-methoxy-
RN: 1984-65-2 **MP** (°C)**:** 31
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.908E-04	1.400E-01	25	L348	1 2 2 1 2	

1077. $C_7H_6Cl_2O$
2,3-Dichloroanisole
1,2-Dichloro-3-methoxybenzene
RN: 1984-59-4 **MP** (°C)**:** 32
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.909E-04	8.690E-02	25	L348	1 2 2 1 2	

1078. $C_7H_6Cl_2O$
2,6-Dichloro-4-methyl-phenol
2,4-Dichloro-6-methyl-phenol-
RN: 2432-12-4 **MP** (°C)**:**
MW: 177.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	2.833E-01	25	B316	0 0 0 0 0	
3.800E-03	6.727E-01	25	B316	0 0 0 0 0	

1079. $C_7H_6N_2O_2S$
p-Cyanobenzenesulfonamide
4-Cyanobenzenesulfonamide
RN: 3119-02-6 **MP** (°C)**:**
MW: 182.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-03	1.111E+00	15	K024	1 2 1 1 2	

1080. $C_7H_6N_2O_4$
2,4-Dinitrotoluene
2,4-Dinitro-toluol
RN: 121-14-2 **MP** (°C)**:** 71
MW: 182.14 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-03	2.709E-01	20	T301	1 2 2 2 2	
1.482E-03	2.699E-01	22	D070	1 2 0 0 1	
1.482E-03	2.700E-01	22	F300	1 0 0 0 1	
1.482E-03	2.699E-01	22	L053	1 1 0 0 1	
2.031E-03	3.699E-01	50	D070	1 2 0 0 1	
2.031E-03	3.699E-01	50	L053	1 1 0 0 1	
1.391E-02	2.534E+00	100	D070	1 2 0 0 2	
1.449E-02	2.640E+00	100	F300	1 0 0 0 2	
1.391E-02	2.534E+00	100	L053	1 1 0 0 2	

1081. $C_7H_6N_2O_5$
2,4-Dinitroanisole
Dinitroanisole
Benzene, 1-methoxy-2,4-dinitro-
RN: 119-27-7 **MP** (°C)**:** 88
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.822E-04	1.550E-01	15	D079	1 2 0 0 2	
6.863E-04	1.360E-01	50	D079	1 2 0 0 2	
2.401E-02	4.757E+00	100	D079	1 2 0 0 2	

1082. $C_7H_6N_2O_5$
Dinitrocresol
DNOC
2,4-Dinitro-6-methylphenol
Dinitro-*o*-cresol
RN: 534-52-1 **MP** (°C)**:** 86
MW: 198.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.561E-04	1.300E-01	15	M161	1 0 0 0 2	
6.309E-04	1.250E-01	ns	B185	0 0 0 0 0	
6.459E-04	1.280E-01	ns	M061	0 0 0 0 2	
1.000E-03	1.981E-01	ns	M163	0 0 0 0 0	EFG
1.262E-03	2.500E-01	ns	N013	0 0 0 0 2	

1083. $C_7H_6N_2S$
4-Thiocyanoaniline
Rhodan
RN: 2987-46-4 **MP** (°C)**:** 142
MW: 150.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	2.000E-01	ns	M061	0 0 0 0 0	

1084. $C_7H_6N_4$
4-Methylpteridine
Pteridine, 4-methyl-
RN: 2432-21-5 **MP** (°C)**:** 151
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.258E-01	4.762E+01	20	A083	1 2 0 0 0	

1085. $C_7H_6N_4$
7-Methylpteridine
Pteridine, 7-methyl-
RN: 936-40-3 **MP** (°C)**:** 196.5
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.775E-01	1.429E+02	20	A083	1 2 0 0 0	

1086. $C_7H_6N_4$
2-Methylpteridine
Pteridine, 2-methyl-
RN: 2432-20-4 **MP** (°C)**:** 140
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-01	1.000E+02	20	A083	1 2 0 0 0	

1087. $C_7H_6N_4O$
2-Methoxypteridine
Pteridine, 2-methoxy-
RN: 102170-44-5 **MP** (°C)**:** 150
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
1.233E+00	2.000E+02	100	A019	1 2 1 1 0	

1088. $C_7H_6N_4O$
4-Hydroxy-6-methylpteridine
4-Pteridinol, 6-methyl-
RN: 16041-24-0 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-02	3.623E+00	20	A019	2 2 1 1 2	
1.341E-01	2.174E+01	100	A019	1 2 1 1 1	

1089. $C_7H_6N_4O$
4-Hydroxy-7-methylpteridine
4-Pteridinol, 7-methyl-
RN: 34244-80-9 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.729E-02	4.425E+00	20	A019	2 2 1 1 2	
1.713E-01	2.778E+01	100	A019	1 2 1 1 1	

1090. $C_7H_6N_4O$
4-Methoxypteridine
Pteridine, 4-methoxy-
RN: 30564-38-6 **MP** (°C)**:** 195
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1091. $C_7H_6N_4O$
7-Methoxypteridine
Pteridine, 7-methoxy-
RN: 204443-27-6 **MP** (°C)**:**
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-01	1.961E+01	20	A083	1 2 0 0 0	
1.233E+00	2.000E+02	100	A083	1 2 0 0 0	

1092. $C_7H_6N_4O$
3,4-Dihydro-4-keto-3-methylpteridine
3:4-Dihydro-4-keto-3-methylpteridine
RN: 24851-65-8 **MP** (°C)**:** 286
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.686E-02	1.408E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1093. $C_7H_6N_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-acetyl-1,5-dihydro-
RN: 96448-60-1 **MP** (°C)**:**
MW: 178.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.210E-03	7.500E-01	22	B428	1 2 1 2 1	

1094. $C_7H_6N_4S$
7-Methylthiopteridine
Pteridine, 7-(methylthio)-
Pteridine-7-methyl-thiol
RN: 204443-30-1 **MP** (°C)**:**
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.792E-02	4.975E+00	20	A083	1 2 0 0 0	
1.439E-01	2.564E+01	100	A083	1 2 0 0 0	

1095. $C_7H_6N_4S$
4-Methylthiopteridine
Pteridine, 4-(methylthio)-
Pteridine-4-methyl-thiol
RN: 6966-78-5 **MP** (°C)**:** 191
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.313E-03	7.686E-01	20	A083	1 2 0 0 0	
3.100E-02	5.525E+00	100	A083	1 2 0 0 0	

1096. $C_7H_6N_4S$
4-Mercapto-7-methylpteridine
4-Pteridinethiol, 7-methyl-
RN: 98550-33-5 **MP** (°C)**:**
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.738E-03	6.662E-01	100	A083	1 2 0 0 0	

1097. $C_7H_6N_4S$
2-Methylthiopteridine
Pteridine, 2-(methylthio)-
Pteridine-2-methyl-thiol
RN: 16878-77-6 **MP** (°C)**:** 136
MW: 178.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.748E-02	3.115E+00	20	A083	1 2 0 0 0	
1.369E-01	2.439E+01	100	A083	1 2 0 0 0	

1098. C_7H_6O
Benzaldehyde
Benzaldehyd
RN: 100-52-7 **MP** (°C)**:** –55
MW: 106.13 **BP** (°C)**:** 179

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.251E-02	3.450E+00	20	C008	1 2 2 0 2	
2.827E-02	3.000E+00	20	F300	1 0 0 0 0	
3.754E-02	3.984E+00	25	B019	1 0 1 2 0	
3.754E-02	3.984E+00	25	B092	2 1 1 1 1	
6.549E-02	6.950E+00	25	C005	2 2 2 2 2	average
3.289E-02	3.490E+00	25	C008	1 2 2 0 2	
6.170E-02	6.548E+00	25	M017	1 2 0 1 2	
3.741E-02	3.970E+00	30	C008	1 2 2 0 2	
2.110E-02	2.239E+00	37	E028	1 0 1 1 2	
8.960E-02	9.509E+00	60	B092	2 0 1 1 1	

1099. $C_7H_6O_2$
Benzoic acid
Benzenecarboxylic acid
Benzoesaeure
RN: 65-85-0 **MP** (°C)**:** 122
MW: 122.12 **BP** (°C)**:** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-02	1.697E+00	0	F302	1 0 0 0 2	
1.390E-02	1.697E+00	0	M043	1 0 0 0 1	
1.720E-02	2.100E+00	10	F300	1 0 0 0 1	
1.716E-02	2.096E+00	10	F302	1 0 0 0 2	
1.634E-02	1.996E+00	10	M043	1 0 0 0 1	
2.010E-02	2.455E+00	15	P329	0 0 0 0 0	
1.982E-02	2.421E+00	15.5	K062	2 0 1 1 2	
2.200E-02	2.687E+00	17	B109	1 0 0 0 2	unit assumed, *sic*
2.237E-02	2.732E+00	17.7	K062	2 0 1 1 2	
2.260E-02	2.760E+00	18	B109	1 0 0 0 2	unit assumed, *sic*
2.211E-02	2.700E+00	18	F071	1 1 2 1 2	
2.100E-02	2.565E+00	18	H009	2 1 2 2 0	EFG, 0.01N HCl
2.211E-02	2.700E+00	18	H080	1 0 0 0 2	
2.257E-02	2.756E+00	18	L050	2 0 1 2 2	
2.211E-02	2.700E+00	18	M344	1 0 0 0 2	
2.308E-02	2.819E+00	19.0	K062	2 0 1 1 2	average of 2
2.368E-02	2.892E+00	20	D041	1 0 0 0 1	
2.339E-02	2.857E+00	20	F069	2 2 2 2 2	
2.375E-02	2.900E+00	20	F300	1 0 0 0 1	
2.368E-02	2.892E+00	20	F302	1 0 0 0 2	
2.200E-02	2.686E+00	20	M038	2 2 1 1 2	
2.368E-02	2.892E+00	20	M043	1 0 0 0 1	
2.457E-02	3.000E+00	20	M049	1 0 0 0 1	
2.400E-02	2.931E+00	20	P329	0 0 0 0 0	
2.825E-02	3.450E+00	20	W026	1 0 1 1 1	average of 2
2.540E-02	3.102E+00	22	E045	2 0 1 1 2	
2.605E-02	3.181E+00	23	E045	2 0 1 1 2	
2.807E-02	3.428E+00	24.6	W029	1 2 1 1 2	
2.620E-02	3.200E+00	25	A412	1 0 2 2 1	int
2.449E-02	2.991E+00	25	B019	1 0 1 2 0	
2.751E-02	3.359E+00	25	B085	2 1 1 1 2	
2.683E-02	3.277E+00	25	B097	2 2 1 1 2	0.01M sodium benzoate
2.800E-02	3.420E+00	25	B128	1 0 1 1 2	
2.768E-02	3.381E+00	25	B302	1 0 0 0 0	pH 2.0
2.805E-02	3.426E+00	25	D058	1 0 1 1 2	
2.746E-02	3.354E+00	25	E045	2 0 1 1 2	
2.810E-02	3.432E+00	25	F001	1 0 1 2 2	
2.784E-02	3.400E+00	25	F300	1 0 0 0 1	
2.800E-02	3.419E+00	25	H009	2 1 2 2 0	EFG, 0.01N HCl
2.784E-02	3.400E+00	25	H015	1 0 0 0 1	
2.251E-03	2.749E-01	25	H060	2 0 2 0 2	*sic*
2.760E-02	3.371E+00	25	H071	2 2 2 1 2	
2.800E-02	3.419E+00	25	H084	1 0 0 0 1	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.371E+00	25	K005	1 0 0 1 2	
2.727E-02	3.330E+00	25	K047	1 2 1 2 2	
2.760E-02	3.371E+00	25	K057	2 2 1 1 2	
2.775E-02	3.389E+00	25	K064	2 2 2 1 2	
2.781E-02	3.396E+00	25	L048	1 2 2 1 2	
2.780E-02	3.395E+00	25	L050	2 0 1 2 2	
2.596E-02	3.170E+00	25	L338	1 0 1 1 2	
2.619E-02	3.199E+00	25	M038	2 2 1 1 2	
2.702E-02	3.300E+00	25	M049	1 0 0 0 1	
2.790E-02	3.407E+00	25	M116	2 1 1 1 2	
2.160E-02	2.638E+00	25	M149	2 0 2 2 2	intrinsic
2.900E-02	3.542E+00	25	O007	1 0 2 1 2	
2.268E-02	2.770E+00	25	P037	2 0 1 1 2	
2.807E-02	3.428E+00	25	P314	0 0 0 0 0	
8.820E+00	1.077E+03	25	P329	0 0 0 0 0	
2.793E-02	3.411E+00	25	R016	0 0 0 0 0	
2.781E-02	3.396E+00	25.0	K062	2 0 1 1 2	average of 2
2.700E-02	3.297E+00	25.00	M135	1 2 1 1 2	0.01N sodium benzoate
2.781E-02	3.396E+00	25.2	C096	1 0 0 1 2	
2.833E-02	3.460E+00	26	E045	2 0 1 1 2	
2.890E-02	3.529E+00	26.4	P043	2 0 1 1 2	
3.439E-02	4.200E+00	26.70	L095	2 2 1 1 2	
2.936E-02	3.586E+00	27	E045	2 0 1 1 2	
3.146E-02	3.842E+00	28	D050	1 2 1 2 2	
3.147E-02	3.843E+00	30	B109	1 0 0 0 2	unit assumed, *sic*
3.204E-02	3.913E+00	30	B109	1 0 0 0 2	unit assumed, *sic*
3.306E-02	4.037E+00	30	B118	1 0 0 0 2	
3.000E-02	3.664E+00	30	B142	2 0 1 1 0	EFG, 0.1N H_2SO_4
3.000E-02	3.664E+00	30	C077	0 0 0 0 0	
3.319E-02	4.054E+00	30	D033	2 2 1 2 2	
3.302E-02	4.033E+00	30	D061	1 0 0 0 2	
2.915E-02	3.560E+00	30	F005	1 2 2 2 2	
3.425E-02	4.182E+00	30	F302	1 0 0 0 2	
3.110E-02	3.799E+00	30	M038	2 2 1 1 2	
3.262E-02	3.984E+00	30	M043	1 0 0 0 1	
3.302E-02	4.033E+00	30	S204	2 0 1 0 2	
3.439E-02	4.200E+00	30	W026	1 0 1 1 1	average of 2
3.216E-02	3.927E+00	30.0	K062	2 0 1 1 2	average of 2
3.400E-02	4.152E+00	31	H009	2 1 2 2 0	EFG, 0.01N HCl
3.873E-02	4.730E+00	35	G052	2 1 1 1 2	
3.711E-02	4.532E+00	35	M038	2 2 1 1 2	
4.010E-02	4.897E+00	35	O007	1 0 2 1 2	
3.772E-02	4.607E+00	35	S204	2 0 1 0 2	
3.960E-02	4.836E+00	35.0	K062	2 0 1 1 2	
3.800E-02	4.641E+00	35.00	M135	1 2 1 1 2	0.01N sodium benzoate
4.201E-02	5.131E+00	37	B171	2 0 1 1 2	
3.611E-02	4.410E+00	37	F005	1 2 2 2 2	
4.200E-02	5.129E+00	37	H009	2 1 2 2 0	EFG, 0.01N HCl
3.734E-02	4.560E+00	37	M360	1 2 1 1 2	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.528E-02	5.529E+00	40	D033	2 2 1 2 2	
4.884E-02	5.964E+00	40	F302	1 0 0 0 1	
4.376E-02	5.345E+00	40	M038	2 2 1 1 2	
4.560E-02	5.569E+00	40	M043	1 0 0 0 1	
4.424E-02	5.403E+00	40	S204	2 0 1 0 2	
5.110E-02	6.241E+00	42.4	W029	1 2 1 1 2	
4.774E-02	5.830E+00	45	F005	1 2 2 2 2	
5.000E-02	6.106E+00	45	H009	2 1 2 2 0	EFG, 0.01N HCl
5.282E-02	6.451E+00	45	M038	2 2 1 1 2	
5.254E-02	6.417E+00	45	S204	2 0 1 0 2	
5.324E-02	6.502E+00	45.0	K062	2 0 1 1 2	
5.500E-02	6.717E+00	45.00	M135	1 2 1 1 2	0.01N sodium benzoate
5.463E-02	6.672E+00	45.3	S124	1 0 0 1 1	
6.878E-02	8.400E+00	50	F300	1 0 0 0 1	
6.901E-02	8.428E+00	50	F302	1 0 0 0 2	
2.107E-02	2.573E+00	50	L006	1 0 0 0 2	
6.237E-02	7.617E+00	50	S204	2 0 1 0 2	
8.032E-02	9.809E+00	53.8	S124	1 0 0 1 2	
7.048E-02	8.607E+00	55	S204	2 0 1 0 2	
8.300E-02	1.014E+01	55.40	M135	1 2 1 1 2	0.01N sodium benzoate
8.853E-02	1.081E+01	57.8	W029	1 2 1 1 2	
9.710E-02	1.186E+01	60	F302	1 0 0 0 2	
9.550E-02	1.166E+01	60	L047	1 1 2 1 2	
9.390E-02	1.147E+01	60	M043	1 0 0 0 2	
1.000E-01	1.221E+01	60.20	M135	1 2 1 1 2	0.01N sodium benzoate
1.129E-01	1.378E+01	62.5	S124	1 0 0 1 2	
1.190E-01	1.453E+01	64.60	M135	1 2 1 1 2	0.01N sodium benzoate
1.390E-01	1.698E+01	68.50	M135	1 2 1 1 2	0.01N sodium benzoate
1.527E-01	1.864E+01	69.4	S124	1 0 0 1 2	
1.424E-01	1.739E+01	70	F302	1 0 0 0 2	
1.658E-01	2.025E+01	74.1	W029	1 2 1 1 2	
1.870E-01	2.284E+01	75.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.242E-01	2.739E+01	79.0	S124	1 0 0 1 2	
2.210E-01	2.699E+01	79.30	M135	1 2 1 1 2	0.01N sodium benzoate
2.192E-01	2.676E+01	80	F302	1 0 0 0 2	
2.168E-01	2.648E+01	80	M043	1 0 0 0 2	
2.540E-01	3.102E+01	82.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.567E-01	3.135E+01	82.3	S124	1 0 0 1 2	
2.485E-01	3.035E+01	83.1	W029	1 2 1 1 2	
3.124E-01	3.815E+01	88.3	W029	1 2 1 1 2	
4.211E-01	5.142E+01	88.6	S124	1 0 0 1 2	
3.550E-01	4.335E+01	88.60	M135	1 2 1 1 2	0.01N sodium benzoate
3.564E-01	4.352E+01	90	F302	1 0 0 0 2	
4.342E-01	5.302E+01	91.5	W029	1 2 1 1 2	average of 3
5.214E-01	6.367E+01	95	D041	1 0 0 0 1	
5.208E-01	6.360E+01	95	F300	1 0 0 0 2	
5.214E-01	6.367E+01	95	F302	1 0 0 0 2	
4.977E-01	6.078E+01	95.3	W029	1 2 1 1 2	
5.493E-01	6.708E+01	98.6	W029	1 2 1 1 2	

(*continued*)

1099. $C_7H_6O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.547E-01	5.553E+01	100	M043	1 0 0 0 2	
8.241E-01	1.006E+02	109.4	W029	1 2 1 1 2	
1.399E+00	1.709E+02	116.1	W029	1 2 1 1 2	
2.594E+00	3.168E+02	116.3	W029	1 2 1 1 2	
2.001E+00	2.444E+02	117.2	W029	1 2 1 1 2	
9.000E-04	1.099E-01	ns	D037	1 1 1 1 0	pH 3.0, intrinsic

1100. $C_7H_6O_2$

m-Hydroxybenzaldehyde
3-Hydroxy-benzaldehyd

RN: 100-83-4 **MP** (°C)**:** 104
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.252E-01	2.750E+01	43	F300	1 0 0 0 2	

1101. $C_7H_6O_2$

p-Hydroxybenzaldehyde
4-Hydroxy-benzaldehyd

RN: 123-08-0 **MP** (°C)**:** 213.5
MW: 122.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-01	1.290E+01	30	F300	1 0 0 0 2	

1102. $C_7H_6O_2$

Salicylaldehyde
Salicylaldehyd

RN: 90-02-8 **MP** (°C)**:** –7
MW: 122.12 **BP** (°C)**:** 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-04	8.077E-02	25	K129	2 1 2 2 2	
1.392E-01	1.700E+01	86	F300	1 0 0 0 1	

1103. $C_7H_6O_3$

Salicylic acid
2-Hydroxybenzoic acid
o-Hydroxybenzoic acid

RN: 69-72-7 **MP** (°C)**:** 158
MW: 138.12 **BP** (°C)**:** 211

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.799E-03	9.391E-01	0	C083	1 2 1 1 2	
5.792E-03	8.000E-01	0	F300	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 1	
9.472E-03	1.308E+00	10	B074	1 2 1 2 2	
8.688E-03	1.200E+00	10	F300	1 0 0 0 1	
1.084E-02	1.498E+00	10	M043	1 0 0 0 0	
1.084E-02	1.498E+00	10	M043	1 0 0 0 1	
8.656E-03	1.196E+00	10	N420	0 0 0 0 0	
9.327E-03	1.288E+00	10	W044	1 0 1 0 2	
1.108E-02	1.531E+00	9.99	A341	0 0 0 0 0	
1.009E-02	1.393E+00	12.1	W044	1 0 1 0 2	
1.207E-02	1.667E+00	14.5	D061	1 0 0 0 2	
1.209E-02	1.670E+00	14.50	B118	1 0 0 0 2	unit assumed
1.028E-02	1.420E+00	15	H022	1 2 2 2 2	
1.520E-03	2.100E-01	15	M461	0 0 0 0 0	
9.875E-03	1.364E+00	15	N420	0 0 0 0 0	
1.258E-02	1.737E+00	17	K046	1 0 0 0 2	spray-dried product
1.330E-02	1.837E+00	20	B074	1 2 1 2 2	
1.303E-02	1.800E+00	20	F071	1 1 2 1 2	
1.303E-02	1.800E+00	20	F300	1 0 0 0 1	
1.303E-02	1.800E+00	20	H080	1 0 0 0 2	
1.296E-02	1.790E+00	20	K047	1 2 1 2 2	
1.445E-02	1.996E+00	20	M043	1 0 0 0 1	
1.445E-02	1.996E+00	20	M043	1 0 0 0 0	
1.445E-02	1.996E+00	20	M107	2 2 1 1 0	EFG
1.303E-02	1.800E+00	20	M344	1 0 0 0 2	
1.154E-02	1.594E+00	20	N420	0 0 0 0 0	
1.593E-02	2.200E+00	20	W026	1 0 1 1 1	average of 2
1.330E-02	1.837E+00	20	W044	1 0 1 0 2	
1.520E-02	2.100E+00	21	B331	1 2 2 1 0	pH 7.4
1.390E-02	1.920E+00	22	E045	2 0 1 1 2	
1.470E-02	2.030E+00	23	E045	2 0 1 1 2	
1.474E-02	2.036E+00	23.0	W044	1 0 1 0 2	
1.550E-02	2.141E+00	24	E045	2 0 1 1 2	
1.847E-02	2.551E+00	24.99	A341	0 0 0 0 0	
1.590E-02	2.196E+00	25	B090	1 1 1 1 2	
1.633E-02	2.255E+00	25	C083	1 2 1 1 2	
1.630E-02	2.251E+00	25	E045	2 0 1 1 2	
1.593E-02	2.200E+00	25	H007	0 0 0 0 0	
1.620E-02	2.238E+00	25	H084	1 0 0 0 2	
1.084E-02	1.498E+00	25	H129	1 0 0 1 0	

(*continued*)

1103. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	2.228E+00	25	K040	1 0 2 1 2	
1.634E-02	2.257E+00	25	K053	2 2 2 2 2	
1.620E-02	2.238E+00	25	K057	2 2 1 1 2	
1.601E-02	2.211E+00	25	L050	2 0 1 2 2	
1.665E-03	2.300E-01	25	M461	0 0 0 0 0	
1.370E-02	1.892E+00	25	N420	0 0 0 0 0	
1.680E-02	2.320E+00	25	O007	1 0 2 1 2	
1.621E-02	2.239E+00	25	P314	0 0 0 0 0	
1.491E-02	2.059E+00	25.50	A012	2 2 2 2 2	
1.700E-02	2.348E+00	26	E045	2 0 1 1 2	
1.780E-02	2.459E+00	27	E045	2 0 1 1 2	
1.746E-02	2.411E+00	27	K046	1 0 0 0 2	spray-dried product
1.728E-02	2.387E+00	28	D050	1 2 1 2 2	
1.784E-02	2.464E+00	28.1	W044	1 0 1 0 2	
1.360E-02	1.878E+00	30	A065	2 0 2 2 1	
1.885E-02	2.603E+00	30	B074	1 2 1 2 2	
1.987E-02	2.745E+00	30	B118	1 0 0 0 2	unit assumed
1.750E-02	2.417E+00	30	B142	2 0 1 1 0	EFG, 0.1N H_2SO_4
1.800E-02	2.486E+00	30	C077	0 0 0 0 0	
1.986E-02	2.743E+00	30	D061	1 0 0 0 2	
1.426E-02	1.970E+00	30	F005	1 2 2 2 2	
1.796E-02	2.481E+00	30	H022	1 2 2 2 2	
1.700E-02	2.348E+00	30	K020	1 0 1 1 0	EFG
1.868E-02	2.580E+00	30	K047	1 2 1 2 2	
2.022E-02	2.792E+00	30	M043	1 0 0 0 0	
2.022E-02	2.792E+00	30	M043	1 0 0 0 1	
2.165E-02	2.991E+00	30	M107	2 2 1 1 0	EFG
2.244E-03	3.100E-01	30	M461	0 0 0 0 0	
1.685E-02	2.327E+00	30	N420	0 0 0 0 0	
2.244E-02	3.100E+00	30	W026	1 0 1 1 2	average of 2
1.906E-02	2.633E+00	30	W044	1 0 1 0 2	
2.172E-02	3.000E+00	30.6	P014	2 1 2 2 0	
2.442E-02	3.373E+00	33.99	A341	0 0 0 0 0	
2.201E-02	3.041E+00	34.4	W044	1 0 1 0 2	
2.273E-02	3.140E+00	35	K047	1 2 1 2 2	
2.039E-02	2.816E+00	35	N420	0 0 0 0 0	
2.390E-02	3.301E+00	35	O007	1 0 2 1 2	
1.332E-02	1.840E+00	37	B171	2 0 1 1 2	
1.861E-02	2.570E+00	37	C079	0 0 0 0 0	
1.897E-02	2.620E+00	37	F005	1 2 2 2 2	
2.452E-02	3.386E+00	37	K046	1 0 0 0 2	spray-dried product
1.303E-02	1.800E+00	37	Y421	0 0 0 0 0	
2.590E-02	3.577E+00	38.7	W044	1 0 1 0 2	
2.848E-02	3.934E+00	40	B074	1 2 1 2 2	
2.679E-02	3.700E+00	40	F300	1 0 0 0 1	
2.672E-02	3.690E+00	40	K047	1 2 1 2 2	
3.028E-02	4.182E+00	40	M043	1 0 0 0 1	

(*continued*)

1103. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-02	4.182E+00	40	M043	1 0 0 0 0	
2.884E-02	3.984E+00	40	M107	2 2 1 1 0	EFG
4.561E-03	6.300E-01	40	M461	0 0 0 0 0	
2.502E-02	3.456E+00	40	N420	0 0 0 0 0	
2.719E-02	3.756E+00	40	W044	1 0 1 0 2	
3.167E-02	4.374E+00	43.99	A341	0 0 0 0 0	
3.743E-02	5.170E+00	44.99	A341	0 0 0 0 0	
2.462E-02	3.400E+00	45	F005	1 2 2 2 2	
3.059E-02	4.226E+00	45	N420	0 0 0 0 0	
3.714E-02	5.130E+00	46.99	A341	0 0 0 0 0	
3.562E-02	4.921E+00	47	K046	1 0 0 0 2	spray-dried product
3.681E-02	5.084E+00	48.6	W044	1 0 1 0 2	
4.102E-02	5.665E+00	49.99	A341	0 0 0 0 0	
4.261E-02	5.885E+00	50	B074	1 2 1 2 2	
6.154E-03	8.500E-01	50	M461	0 0 0 0 0	
3.769E-02	5.206E+00	50	N420	0 0 0 0 0	
3.889E-02	5.371E+00	50	W044	1 0 1 0 2	
4.337E-02	5.991E+00	50.99	A341	0 0 0 0 0	
4.677E-02	6.461E+00	51.99	A341	0 0 0 0 0	
5.151E-02	7.115E+00	53.99	A341	0 0 0 0 0	
5.319E-02	7.347E+00	54.99	A341	0 0 0 0 0	
4.947E-02	6.833E+00	56.0	W044	1 0 1 0 2	
6.104E-02	8.431E+00	57.49	A341	0 0 0 0 0	
6.202E-02	8.566E+00	60	B074	1 2 1 2 2	
6.009E-02	8.300E+00	60	F300	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 0	
5.888E-02	8.133E+00	60	W044	1 0 1 0 2	
7.184E-02	9.922E+00	61.49	A341	0 0 0 0 0	
7.140E-02	9.862E+00	64.0	W044	1 0 1 0 2	
8.184E-02	1.130E+01	65.99	A341	0 0 0 0 0	
8.373E-02	1.156E+01	66.0	W044	1 0 1 0 2	
1.252E-01	1.730E+01	75.0	W044	1 0 1 0 2	
1.499E-01	2.070E+01	80	F300	1 0 0 0 2	
1.600E-01	2.210E+01	80	M043	1 0 0 0 0	
1.600E-01	2.210E+01	80	M043	1 0 0 0 2	
5.437E-01	7.510E+01	100	M043	1 0 0 0 0	
5.437E-01	7.510E+01	100	M043	1 0 0 0 2	
1.598E-02	2.207E+00	ns	O003	0 2 1 1 2	
1.514E-02	2.091E+00	ns	R427	0 0 0 0 0	
1.841E-02	2.544E+00	rt	H431	0 0 0 0 0	

1104. $C_7H_6O_3$

Protocatechualdehyde
3,4-Dihydroxy-benzaldehyd
RN: 139-85-5 **MP** (°C)**:**
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.620E-01	5.000E+01	20	F300	1 0 0 0 0	
~1.88E+00	~2.60E+02	100	F300	1 0 0 0 0	

1105. $C_7H_6O_3$

p-Hydroxybenzoic acid
4-Hydroxy-benzoesaeure
4-Hydroxybenzoic acid
p-Hydroxybenzoicacid
4-Hydroxybenzenecarboxylic acid
RN: 99-96-7 **MP** (°C)**:** 214.5
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-02	2.494E+00	0	M043	1 0 0 0 1	
1.590E-02	2.196E+00	4.99	A405	2 0 1 1 2	
2.525E-02	3.488E+00	10	M043	1 0 0 0 1	
2.280E-02	3.149E+00	10.99	A405	2 0 1 1 2	
2.216E-02	3.061E+00	12.7	W044	1 0 1 0 2	
5.746E-02	7.937E+00	15	D041	1 0 0 0 0	
3.186E-02	4.400E+00	15	F300	1 0 0 0 1	
2.624E-02	3.624E+00	15	H022	1 2 2 2 2	
2.990E-02	4.130E+00	15.99	A405	2 0 1 1 2	
3.740E-02	5.166E+00	19.99	A405	2 0 1 1 2	
3.470E-02	4.793E+00	20	C006	1 2 1 1 2	
3.817E-02	5.272E+00	20	M043	1 0 0 0 1	
3.602E-02	4.975E+00	20	M107	2 2 1 1 0	EFG
3.545E-02	4.896E+00	20.9	W044	1 0 1 0 2	
4.890E-02	6.754E+00	24.99	A405	2 0 1 1 2	
3.545E-02	4.896E+00	25	D081	1 1 2 1 2	
6.580E-02	9.089E+00	25	D339	0 0 0 0 0	
4.634E-02	6.400E+00	25	H007	0 0 0 0 0	
3.318E-02	4.583E+00	25	M334	1 2 1 1 2	
4.322E-02	5.970E+00	25	N023	1 2 2 1 2	hydrate
6.241E-02	8.620E+00	25	N023	1 2 2 1 2	anhydrate
3.873E-02	5.350E+00	25.50	A012	2 2 2 2 2	
6.340E-02	8.757E+00	29.99	A405	2 0 1 1 2	
5.400E-02	7.459E+00	30	A065	2 0 2 2 1	
4.800E-02	6.630E+00	30	C077	0 0 0 0 0	
5.500E-02	7.597E+00	30	H019	0 0 0 0 0	
5.421E-02	7.488E+00	30	H022	1 2 2 2 2	
5.500E-02	7.597E+00	30	K020	1 0 1 1 0	EFG

(*continued*)

1105. $C_7H_6O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-02	7.937E+00	30	M043	1 0 0 0 1	
5.746E-02	7.937E+00	30	M107	2 2 1 1 0	EFG
5.538E-02	7.650E+00	30	N023	1 2 2 1 2	hydrate
7.790E-02	1.076E+01	30	N023	1 2 2 1 2	anhydrate
5.496E-02	7.592E+00	30	W044	1 0 1 0 2	
8.120E-02	1.122E+01	33.99	A405	2 0 1 1 2	
7.076E-02	9.774E+00	34.4	W044	1 0 1 0 2	
7.247E-02	1.001E+01	35	N023	1 2 2 1 2	hydrate
9.781E-02	1.351E+01	35	N023	1 2 2 1 2	anhydrate
1.231E-01	1.700E+01	37	B171	2 0 1 1 2	
1.027E-01	1.419E+01	38.99	A405	2 0 1 1 2	
8.663E-02	1.197E+01	39.4	W044	1 0 1 0 2	
8.938E-02	1.235E+01	40	M043	1 0 0 0 2	
9.996E-02	1.381E+01	40	M107	2 2 1 1 0	EFG
1.203E-01	1.662E+01	40	N023	1 2 2 1 2	anhydrate
9.339E-02	1.290E+01	40	N023	1 2 2 1 2	hydrate
1.385E-01	1.913E+01	42.99	A405	2 0 1 1 2	
1.291E-01	1.783E+01	46.0	W044	1 0 1 0 2	
1.804E-01	2.492E+01	47.99	A405	2 0 1 1 2	
2.438E-01	3.367E+01	52.99	A405	2 0 1 1 2	
1.931E-01	2.667E+01	54.6	W044	1 0 1 0 2	
3.330E-01	4.600E+01	56.99	A405	2 0 1 1 2	
2.978E-01	4.114E+01	60	M043	1 0 0 0 2	
4.286E-01	5.920E+01	61.99	A405	2 0 1 1 2	
5.666E-01	7.826E+01	66.99	A405	2 0 1 1 2	
7.269E-01	1.004E+02	71.99	A405	2 0 1 1 2	
1.835E-01	2.534E+01	75	D041	1 0 0 0 1	
8.723E-01	1.205E+02	80	M043	1 0 0 0 2	
1.875E+00	2.590E+02	100	F300	1 0 0 0 2	
2.410E+00	3.329E+02	100	M043	1 0 0 0 2	
3.715E-02	5.132E+00	ns	R427	0 0 0 0 0	
4.854E-02	6.705E+00	rt	H431	0 0 0 0 0	

1106. $C_7H_6O_3$

β-2-Furyncrylic acid
β-2-Furylacrylic acid
β-Furyl-(2)-acrylsaeure

RN: 539-47-9 **MP** (°C)**:** 143
MW: 138.12 **BP** (°C)**:** 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.448E-02	2.000E+00	20	F300	1 0 0 0 0	

1107. $C_7H_6O_3$

m-Hydroxybenzoic acid
3-Hydroxy-benzoesaeure
3-Hydroxybenzoic acid
m-Hydroxybenzoicacid

RN: 99-06-9 **MP** (°C)**:** 202
MW: 138.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	3.488E+00	0	M043	1 0 0 0 1	
3.960E-02	5.470E+00	10	M043	1 0 0 0 1	
4.804E-02	6.636E+00	13.3	W044	1 0 1 0 2	
5.068E-02	7.000E+00	15	F300	1 0 0 0 1	
4.477E-02	6.184E+00	15	H022	1 2 2 2 2	
6.052E-02	8.360E+00	18.8	W044	1 0 1 0 2	
6.173E-02	8.527E+00	20	M043	1 0 0 0 1	
4.318E-02	5.964E+00	20	M107	2 2 1 1 0	EFG
7.551E-02	1.043E+01	24.3	W044	1 0 1 0 2	
5.249E-02	7.250E+00	25.50	A012	2 2 2 2 2	
7.800E-03	1.077E+00	30	A065	2 0 2 2 1	
8.600E-02	1.188E+01	30	C077	0 0 0 0 0	
8.800E-02	1.215E+01	30	H019	0 0 0 0 0	
8.300E-02	1.146E+01	30	H021	1 2 1 1 0	EFG
9.291E-02	1.283E+01	30	M043	1 0 0 0 1	
6.813E-02	9.411E+00	30	M107	2 2 1 1 0	EFG
9.552E-02	1.319E+01	30	W044	1 0 1 0 2	
9.855E-02	1.361E+01	30.9	W044	1 0 1 0 2	
1.271E-01	1.756E+01	36.2	W044	1 0 1 0 2	
1.420E-01	1.961E+01	40	M043	1 0 0 0 1	
1.105E-01	1.526E+01	40	M107	2 2 1 1 0	EFG
2.809E-01	3.880E+01	50	F300	1 0 0 0 1	
2.222E-01	3.070E+01	51.0	W044	1 0 1 0 2	
3.118E-01	4.306E+01	60	M043	1 0 0 0 1	
7.987E-01	1.103E+02	80	M043	1 0 0 0 2	
2.678E+00	3.699E+02	100	M043	1 0 0 0 2	
1.810E-02	2.500E+00	ns	B361	0 0 0 0 0	
5.012E-02	6.923E+00	ns	R427	0 0 0 0 0	

1108. $C_7H_6O_4$

2,6-Dihydroxybenzoic acid
2,6-Dihydroxy-benzoesaeure
γ-Resorcylic acid

RN: 303-07-1 **MP** (°C)**:**
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-02	9.556E+00	ns	C014	0 0 0 1 1	

1109. $C_7H_6O_4$
Protocatechuic acid
3,4-Dihydroxy-benzoesaeure
3,4-Dihydroxybenzoic acid
RN: 99-50-3 **MP** (°C)**:**
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.181E-01	1.820E+01	14	F300	1 0 0 0 2	
1.440E+00	2.220E+02	80	F300	1 0 0 0 2	

1110. $C_7H_6O_4$
β-Resorcyclic acid
2,4-Dihydroxy-benzoesaeure
2,4-Dihydroxybenzoic acid
2,4-Dihydroxybenzoicacid
β-Resorcylic acid
4-Hydroxysalicylic acid
RN: 89-86-1 **MP** (°C)**:** 225
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.893E-02	6.000E+00	25	H007	0 0 0 0 0	

1111. $C_7H_6O_4$
Gentisic acid
2,5-Dihydroxy-benzoesaeure
2,5-Dihydroxybenzoic acid
2,5-Dihydroxybenzoicacid
Hydroquinonecarboxylic acid
RN: 490-79-9 **MP** (°C)**:** 205
MW: 154.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-01	2.200E+01	25	H007	0 0 0 0 0	

1112. $C_7H_6O_5$
Gallic acid
3,4,5-Trihydroxybenzoesaeure
Gallussaeure
RN: 149-91-7 **MP** (°C)**:** 250
MW: 170.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E+00	2.253E+02	–10.0	L430	0 0 0 0 0	
5.349E-02	9.100E+00	15	M461	0 0 0 0 0	
5.589E-02	9.509E+00	19.99	L430	0 0 0 0 0	

(*continued*)

1112. $C_7H_6O_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.995E-02	1.190E+01	20	F300	1 0 0 0 2	
5.820E-02	9.901E+00	24.99	L430	0 0 0 0 0	
8.641E-02	1.470E+01	25	M461	0 0 0 0 0	
8.001E-02	1.361E+01	29.99	L430	0 0 0 0 0	
1.093E-01	1.860E+01	30	M461	0 0 0 0 0	
1.034E-01	1.759E+01	34.99	L430	0 0 0 0 0	
1.355E-01	2.306E+01	39.99	L430	0 0 0 0 0	
1.552E-01	2.640E+01	40	M461	0 0 0 0 0	
1.751E-01	2.979E+01	44.99	L430	0 0 0 0 0	
2.272E-01	3.865E+01	49.99	L430	0 0 0 0 0	
2.240E-01	3.810E+01	50	M461	0 0 0 0 0	
2.879E-01	4.898E+01	54.99	L430	0 0 0 0 0	
3.774E-01	6.420E+01	59.99	L430	0 0 0 0 0	
4.470E-01	7.604E+01	64.99	L430	0 0 0 0 0	
6.044E-01	1.028E+02	69.99	L430	0 0 0 0 0	
7.064E-01	1.202E+02	74.99	L430	0 0 0 0 0	
9.497E-01	1.616E+02	79.99	L430	0 0 0 0 0	
1.198E+00	2.038E+02	84.99	L430	0 0 0 0 0	
1.505E+00	2.561E+02	100	F300	1 0 0 0 2	
4.202E-02	7.149E+00	–.0	L430	0 0 0 0 0	
6.918E-02	1.177E+01	ns	R427	0 0 0 0 0	

1113. $C_7H_6O_5$

2,3,4-Trihydroxybenzoic acid
2,3,4-Trihydroxybenzoesaeure

RN: 610-02-6 **MP** (°C)**:**
MW: 170.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.878E-03	1.000E+00	12.50	F300	1 0 0 0 0	

1114. C_7H_7Br

m-Bromotoluene
3-Bromotoluene
3-Methyl-1-bromobenzene
1-Bromo-3-methylbenzene
3-Bromo-1-methylbenzene
3-Methylphenyl bromide

RN: 591-17-3 **MP** (°C)**:** –39.8
MW: 171.04 **BP** (°C)**:** 183.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	5.131E-02	ns	O013	0 1 0 1 0	
3.020E-04	5.165E-02	ns	S460	0 0 0 0 0	

1115. C_7H_7Cl

m-Chlorotoluene
3-Chlorotoluene
1-Chloro-3-methylbenzene
m-Tolyl chloride

RN: 108-41-8 **MP** (°C)**:** –48
MW: 126.59 **BP** (°C)**:** 161.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1116. C_7H_7Cl

o-Chlorotoluene
2-Chlorotoluene
2-Chloro-1-methylbenzene
2-Methylchlorobenzene
1-Methyl-2-chlorobenzene
OCT

RN: 95-49-8 **MP** (°C)**:** –36
MW: 126.59 **BP** (°C)**:** 159.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1117. C_7H_7Cl

p-Chlorotoluene
4-Chlorotoluene
p-Tolyl chloride
4-Chloro-1-methyl-benzene
PCT
1-Chloro-4-methylbenzene

RN: 106-43-4 **MP** (°C)**:** 8
MW: 126.59 **BP** (°C)**:** 162.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-04	1.065E-01	20	H118	1 1 1 1 2	
1.084E-03	1.372E-01	20	H301	0 0 0 0 0	
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1118. $C_7H_7ClN_2O_4S$

Saluamine
2-Amino-4-chloro-5-sulfamoylbenzoic acid
4-Chloro-5-sulfamylanthranilic acid
Desfurylmethylfurosemide
4-Chloro-5-sulfamoylanthranilic acid
-Amino-5-aminosulfonyl-4-chlorobenzoic acid
RN: 3086-91-7 **MP** (°C)**:**
MW: 250.66 **BP** (°C)**:** 549.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.218E-03	5.560E-01	25	B405	1 1 1 2 2	Buffer pH 2.0
3.008E-03	7.540E-01	25	B405	1 1 1 2 2	

1119. $C_7H_7ClN_4O_2$

8-Chlorotheophylline
8-Chloro-1,3-dimethyl-2,6(1H,3H)-purinedione
RN: 85-18-7 **MP** (°C)**:** 290
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.481E-01	ns	R427	0 0 0 0 0	

1120. C_7H_7ClO

Chlorocresol
3-Methyl-4-chlorophenol
4-Chloro-3-cresol
6-Chloro-3-hydroxytoluene
3-Methyl-4-chloro-phenol-
Phenol, 4-chloro-3-methyl-
RN: 59-50-7 **MP** (°C)**:** 67
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	3.992E+00	25	B316	0 0 0 0 0	
3.489E-02	4.975E+00	25	R041	0 0 0 0 0	
3.647E-02	5.200E+00	ns	G024	0 0 0 0 2	

1121. C_7H_7ClO

4-Chloroanisole
p-Chloroanisole
1-Chloro-4-methoxybenzene
RN: 623-12-1 **MP** (°C)**:** –18
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.662E-03	2.370E-01	25	L348	1 2 2 1 2	

1122. C_7H_7ClO

2-Methyl-6-chloro-phenol
2-Chloro-6-methylphenol
6-Chloro-*o*-cresol
3-Chloro-2-hydroxytoluene
6-Chloro-2-methylphenol

RN: 87-64-9 **MP** (°C)**:**
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.565E+00	25	B316	0 0 0 0 0	

1123. C_7H_7ClO

2-Methyl-4-chloro-phenol
4-Chloro-*o*-cresol
4-Chloro-2-methylphenol
5-Chloro-2-hydroxytoluene

RN: 1570-64-5 **MP** (°C)**:** 45–48
MW: 142.59 **BP** (°C)**:** 220–225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-02	6.844E+00	25	B316	0 0 0 0 0	

1124. C_7H_7ClO

2-Chloroanisole
o-Chloroanisole

RN: 766-51-8 **MP** (°C)**:** –27
MW: 142.59 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.437E-03	4.900E-01	25	L348	1 2 2 1 2	
3.467E-03	4.944E-01	ns	S460	0 0 0 0 0	

1125. C_7H_7ClO

3-Chloroanisole
m-Chloroanisole
1-Chloro-3-methoxybenzene

RN: 2845-89-8 **MP** (°C)**:** <25
MW: 142.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-03	2.350E-01	25	L348	1 2 2 1 2	
1.660E-03	2.366E-01	ns	S460	0 0 0 0 0	

1126. $C_7H_7Cl_2NO$

Clopidol
3,5-Dichloro-2,6-dimethyl-4-pyridinol
Coyden
Methylchloropindol
RN: 2971-90-6 **MP** (°C)**:**
MW: 192.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-04	4.000E-02	ns	K138	0 0 0 0 1	

1127. $C_7H_7Cl_3NO_3PS$

Chlorpyrifos-methyl
Chlorpyrifos-methy
RN: 5598-13-0 **MP** (°C)**:**
MW: 322.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
9.922E-06	3.200E-03	20	B300	2 1 1 1 2	
9.922E-06	3.200E-03	20	B324	0 0 0 0 0	
9.921E-06	3.200E-03	20	B324	0 0 0 0 0	
1.476E-05	4.760E-03	20	C053	0 0 0 0 0	
1.240E-05	4.000E-03	24	K069	2 0 0 1 1	
1.240E-05	4.000E-03	25	M161	1 0 0 0 0	
2.139E-05	6.899E-03	30	B324	0 0 0 0 0	
2.139E-05	6.900E-03	30	B324	0 0 0 0 0	
1.476E-05	4.760E-03	ns	F071	0 1 2 1 2	
1.240E-05	4.000E-03	ns	K138	0 0 0 0 1	
1.643E-05	5.300E-03	ns	M110	0 0 0 0 0	EFG

1128. $C_7H_7Cl_3NO_4P$

Torelle
Dimethyl 3,5,6-trichloro-2-pyridinyl phosphate
DOWCO 217
Fospirate
Phosphoric acid, dimethyl 3,5,6-trichloro-2-pyridyl ester
RN: 5598-52-7 **MP** (°C)**:**
MW: 306.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.789E-04	3.000E-01	24	K069	2 0 0 1 1	

1129. $C_7H_7FN_2O_3$
3-Propionyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Propionyl-5-fluorouracil
RN: 75410-16-1 **MP** (°C)**:** 113–114
MW: 186.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-01	3.530E+01	22	B321	0 0 0 0 0	pH 4.0
1.896E-01	3.530E+01	22	B332	1 1 0 0 1	pH 4.0
1.980E-01	3.686E+01	22	B416	2 2 1 2 1	

1130. $C_7H_7FN_2O_4$
3-Acetoxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Acetoxymethyl-5-fluorouracil
RN: 73042-04-3 **MP** (°C)**:** 158–159
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.894E-02	2.000E+01	22	B321	0 0 0 0 0	pH 4.0

1131. $C_7H_7FN_2O_4$
1-Acetoxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Acetoxymethyl-5-fluorouracil
RN: 62113-41-1 **MP** (°C)**:** 122–123
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.132E-01	4.310E+01	22	B321	0 0 0 0 0	pH 4.0

1132. $C_7H_7FN_2O_4$
3-Ethyloxycarbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Ethyloxycarbonyl-5-fluorouracil
1-Ethyloxycarbonyl-5-fluorouracil
RN: 75410-27-4 **MP** (°C)**:** 126–128
MW: 202.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E-01	7.200E+01	22	B321	0 0 0 0 0	pH 4.0
3.413E-02	6.900E+00	22	B332	1 1 0 0 1	pH 4.0

1133. C_7H_7NO

Benzamide
Benzamid
Phenyl carboxamide
Benzoic acid amide

RN: 55-21-0 **MP** (°C)**:** 130
MW: 121.14 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.923E-02	5.964E+00	10	M043	1 0 0 0 0	
4.750E-02	5.754E+00	12	O019	1 0 0 1 2	
1.000E-01	1.211E+01	20	B139	2 1 1 1 1	
8.173E-02	9.901E+00	20	M043	1 0 0 0 1	
1.100E-01	1.333E+01	22	J037	0 0 0 0 0	
1.106E-01	1.340E+01	25	F300	1 0 0 0 2	
1.059E-01	1.283E+01	30	M043	1 0 0 0 1	
1.300E-01	1.575E+01	40	M043	1 0 0 0 1	
1.651E-01	2.000E+01	50	P064	2 0 1 1 1	
3.931E-01	4.762E+01	60	M043	1 0 0 0 0	
6.191E-01	7.500E+01	70	P064	2 0 1 1 1	
5.503E+00	6.667E+02	80	M043	1 0 0 0 2	
6.686E+00	8.100E+02	90	P064	2 0 1 1 2	
7.338E+00	8.889E+02	100	M043	1 0 0 0 2	
7.842E+00	9.500E+02	110	P064	2 0 1 1 2	
1.100E-01	1.332E+01	rt	D021	0 0 1 1 2	

1134. $C_7H_7NO_2$

Salicylamide
2-Hydroxybenzoicacidamide
Algamon
Amid-sal
Amidosal
Algiamida

RN: 65-45-2 **MP** (°C)**:** 140
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.878E-03	1.218E+00	10	N419	0 0 0 0 0	
1.060E-02	1.454E+00	15	D012	1 1 0 1 2	
1.137E-02	1.559E+00	15	N419	0 0 0 0 0	
1.100E-02	1.509E+00	16	D012	1 1 0 1 2	
1.531E-02	2.100E+00	20	E046	1 0 0 0 0	EFG
1.447E-02	1.985E+00	20	N419	0 0 0 0 0	
1.900E-02	2.606E+00	22	J031	0 0 0 0 0	
1.604E-02	2.200E+00	23	B328	1 2 2 1 1	pH 4.0
1.500E-02	2.057E+00	25	D012	1 1 0 1 2	
1.750E-02	2.400E+00	25	E046	1 0 0 0 0	EFG
1.757E-02	2.409E+00	25	N419	0 0 0 0 0	
1.831E-02	2.511E+00	25	P314	0 0 0 0 0	

(*continued*)

1134. $C_7H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.115E-02	2.900E+00	30	E046	1 0 0 0 0	EFG
2.166E-02	2.970E+00	30	N419	0 0 0 0 0	
2.771E-02	3.800E+00	35	E046	1 0 0 0 0	EFG
2.685E-02	3.682E+00	35	N419	0 0 0 0 0	
2.900E-02	3.977E+00	37	D012	1 1 0 1 2	
3.427E-02	4.700E+00	40	E046	1 0 0 0 0	EFG
3.285E-02	4.505E+00	40	N419	0 0 0 0 0	
4.280E-02	5.870E+00	45	D012	1 1 0 1 2	
4.181E-02	5.734E+00	45	N419	0 0 0 0 0	
5.323E-02	7.300E+00	50	E046	1 0 0 0 0	EFG
5.371E-02	7.366E+00	50	N419	0 0 0 0 0	
1.677E-03	2.300E-01	ns	B361	0 0 0 0 0	

1135. $C_7H_7NO_2$

p-Aminobenzoic acid
4-Amino-benzoesaeure
4-Aminobenzoic acid
p-Aminobenzoicacid
1-Amino-4-carboxybenzene

RN: 150-13-0 **MP** (°C)**:** 187.0
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.479E-02	3.400E+00	12.80	F300	1 0 0 0 1	
3.609E-02	4.950E+00	18	C033	1 0 2 1 2	
3.628E-02	4.975E+00	25	D041	1 0 0 0 0	
3.930E-02	5.390E+00	25	L338	1 0 1 1 2	
3.646E-02	5.000E+00	25	M054	1 0 0 0 0	
3.500E-02	4.800E+00	25	P015	0 0 0 0 0	
4.455E-02	6.110E+00	30	C033	1 0 2 1 2	
4.579E-02	6.280E+00	30	H018	0 0 0 0 0	
4.500E-02	6.171E+00	30	L069	1 0 1 1 0	EFG
6.125E-02	8.400E+00	37	B171	2 0 1 1 2	
6.040E-02	8.283E+00	37	F006	1 1 2 2 2	

1136. $C_7H_7NO_2$

o-Nitrotoluene
2-Nitro-toluol
2-Nitrotoluene

RN: 88-72-2 **MP** (°C)**:** –9.5
MW: 137.14 **BP** (°C)**:** 221.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.872E-03	5.310E-01	9.99	B403	1 2 2 2 2	
4.441E-03	6.090E-01	19.99	B403	1 2 2 2 2	

(*continued*)

1136. $C_7H_7NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.017E-03	6.880E-01	29.99	B403	1 2 2 2 2	
4.740E-03	6.500E-01	30	F300	1 0 0 0 2	
5.637E-03	7.730E-01	39.99	B403	1 2 2 2 2	

1137. $C_7H_7NO_2$

o-Aminobenzoic acid
2-Aminobenzoic acid
Anthranilsaeure

RN: 118-92-3 **MP** (°C)**:** 145
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.181E-02	2.991E+00	10	M043	1 0 0 0 0	
2.543E-02	3.488E+00	14	D041	1 0 0 0 1	
2.552E-02	3.500E+00	14	F300	1 0 0 0 1	
2.543E-02	3.488E+00	20	M043	1 0 0 0 1	
4.349E-02	5.964E+00	30	M043	1 0 0 0 0	
6.504E-02	8.920E+00	40	M043	1 0 0 0 0	
3.552E+00	4.872E+02	100	M043	1 0 0 0 1	

1138. $C_7H_7NO_2$

m-Nitrotoluene
3-Nitro-toluol
3-Nitrotoluene

RN: 99-08-1 **MP** (°C)**:** 16
MW: 137.14 **BP** (°C)**:** 232.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.281E-03	4.500E-01	9.99	B403	1 2 2 2 2	
3.580E-03	4.910E-01	19.99	B403	1 2 2 2 2	
3.894E-03	5.340E-01	29.99	B403	1 2 2 2 2	
3.646E-03	5.000E-01	30	F300	1 0 0 0 2	
4.120E-03	5.650E-01	39.99	B403	1 2 2 2 2	

1139. $C_7H_7NO_2$

m-Aminobenzoic acid
3-Amino-benzoesaeure
3-Aminobenzoic acid

RN: 99-05-8 **MP** (°C)**:** 174
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	5.900E+00	14.90	F300	1 0 0 0 1	
5.830E-02	7.995E+00	30	W007	2 0 2 2 2	

1140. $C_7H_7NO_2$
Methyl nicotinate
Nicotinsaeure-methyl ester
RN: 93-60-7 **MP** (°C)**:** 39
MW: 137.14 **BP** (°C)**:** 209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.471E-01	4.760E+01	20	F300	1 0 0 0 2	*sic*
8.065E+00	1.106E+03	32	L346	1 0 0 1 0	
3.467E-01	4.755E+01	ns	R424	0 0 0 0 0	

1141. $C_7H_7NO_2$
p-Nitrotoluene
4-Nitrotoluene
RN: 99-99-0 **MP** (°C)**:** 55
MW: 137.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	1.790E-01	9.99	B403	1 2 2 2 2	
2.917E-04	4.000E-02	14.5	D070	1 2 0 0 1	
2.917E-04	4.000E-02	14.50	F300	1 0 0 0 1	
1.765E-03	2.420E-01	19.99	B403	1 2 2 2 2	
2.100E-03	2.880E-01	20	H306	1 0 1 2 1	
2.150E-03	2.949E-01	20	T301	1 2 2 2 2	
2.348E-03	3.220E-01	29.99	B403	1 2 2 2 2	
3.048E-03	4.180E-01	39.99	B403	1 2 2 2 2	
5.687E-04	7.799E-02	50	D070	1 2 0 0 1	
8.458E-04	1.160E-01	100	D070	1 2 0 0 2	

1142. $C_7H_7NO_3$
3-Methyl-4-nitrophenol
3-Nitro-*p*-cresol
3-Nitro-*p*-kresol
4-Nitro-5-methylphenol
RN: 2581-34-2 **MP** (°C)**:** 128
MW: 153.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.769E-03	1.190E+00	25	B104	1 2 1 1 1	
7.762E-03	1.189E+00	ns	R427	0 0 0 0 0	

1143. $C_7H_7NO_3$
p-Aminosalicylic acid
4-Amino-salicylsaeure
4-Aminosalicylic acid
RN: 65-49-6 **MP** (°C)**:** 150
MW: 153.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	1.996E+00	20	D041	1 0 0 0 0	
1.100E-02	1.685E+00	23	M072	1 2 1 1 0	EFG
2.100E-02	3.216E+00	30	L069	1 0 1 1 0	EFG
1.087E-02	1.664E+00	ns	H125	0 0 0 0 0	

1144. $C_7H_7NO_3$
p-Nitroanisol
4-Nitro-anisol
4-Nitroanisol
RN: 100-17-4 **MP** (°C)**:** 54
MW: 153.14 **BP** (°C)**:** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	7.000E-02	15	F300	1 0 0 0 1	
3.853E-03	5.900E-01	30	F300	1 0 0 0 2	

1145. $C_7H_7N_2OS$
Ethyl acetylthiodiazole
Ethyle acetyle thiodiazolique
RN: **MP** (°C)**:**
MW: 167.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-03	2.000E-01	37	D084	1 0 1 0 1	

1146. $C_7H_7N_5$
2-Methylaminopteridine
Pteridine, 2-(methylamino)-
RN: 19167-57-8 **MP** (°C)**:** 219
MW: 161.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-02	3.115E+00	20	A019	2 2 1 1 1	
1.724E-01	2.778E+01	100	A019	1 2 1 1 1	

1147. C_7H_8
Toluene
Methylbenzene
RN: 108-88-3 **MP** (°C)**:** –94
MW: 92.14 **BP** (°C)**:** 110.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.819E-03	5.362E-01	.06	U010	1 0 0 1 1	EFG
7.857E-03	7.240E-01	0	P003	2 2 2 2 2	
6.638E-03	6.116E-01	4.50	B086	2 1 2 2 2	
5.557E-03	5.120E-01	4.62	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	4.62	U013	1 0 0 0 0	EFG
6.519E-03	6.006E-01	6.30	B086	2 1 2 2 2	
6.356E-03	5.857E-01	7.10	B086	2 1 2 2 2	
6.367E-03	5.867E-01	9	B086	2 1 2 2 2	
6.210E-03	5.722E-01	10	B149	2 1 1 2 2	
6.215E-03	5.727E-01	11.80	B086	2 1 2 2 2	
6.237E-03	5.747E-01	12.10	B086	2 1 2 2 2	
5.307E-03	4.890E-01	14.20	U013	1 0 0 0 0	EFG
5.785E-03	5.330E-01	15	S203	1 1 2 1 2	
6.172E-03	5.687E-01	15.10	B086	2 1 2 2 2	
5.424E-03	4.998E-01	16	D052	1 1 0 0 0	
5.100E-03	4.699E-01	16	F001	1 0 1 2 1	
5.101E-03	4.700E-01	16	F071	1 1 2 1 2	
5.101E-03	4.700E-01	16	F300	1 0 0 0 2	
5.101E-03	4.700E-01	16	H080	1 0 0 0 2	
5.100E-03	4.699E-01	16	S006	1 0 0 0 1	
6.370E-03	5.869E-01	20	B149	2 1 1 2 2	
6.154E-03	5.670E-01	20	B356	0 0 0 0 0	
5.424E-03	4.998E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
5.590E-03	5.151E-01	20	M312	1 0 0 0 2	
4.982E-03	4.591E-01	20	M337	2 1 2 2 2	
6.139E-03	5.657E-01	20.10	B086	2 1 2 2 2	
5.196E-03	4.788E-01	21	C024	2 1 1 2 2	
5.752E-03	5.300E-01	25	A001	1 2 2 2 1	
5.098E-03	4.698E-01	25	A094	1 0 0 0 1	
6.805E-03	6.270E-01	25	B003	2 1 2 2 2	
5.589E-03	5.150E-01	25	B060	2 0 1 1 1	
6.690E-03	6.164E-01	25	B153	2 1 1 1 2	
1.680E-02	1.548E+00	25	B173	2 0 2 2 2	*sic*
5.687E-03	5.240E-01	25	B304	2 0 2 2 2	
8.000E-03	7.371E-01	25	H092	1 1 1 1 0	
6.500E-03	5.989E-01	25	H313	2 1 2 2 1	
6.000E-03	5.529E-01	25	H332	2 2 2 2 0	
6.370E-02	5.869E+00	25	I334	2 2 2 1 2	*sic*
6.370E-03	5.869E-01	25	I335	2 2 2 2 2	
5.430E-03	5.003E-01	25	K001	1 0 2 1 2	
5.318E-03	4.900E-01	25	K072	1 0 1 1 1	
6.290E-03	5.796E-01	25	K316	2 2 2 2 2	
5.641E-03	5.197E-01	25	L319	1 0 2 1 2	

(*continued*)

1147. C_7H_8 (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.589E-03	5.150E-01	25	M130	1 0 0 0 2	
5.638E-03	5.195E-01	25	M132	2 2 2 1 2	
6.280E-03	5.787E-01	25	M342	1 0 1 1 2	
6.219E-03	5.730E-01	25	P003	2 2 2 2 2	
6.012E-03	5.540E-01	25	P051	2 1 1 2 2	
6.045E-03	5.570E-01	25	S203	1 1 2 1 2	
5.804E-03	5.348E-01	25	S358	2 1 2 2 2	
5.650E-03	5.206E-01	25	S359	2 1 2 2 2	
6.280E-03	5.787E-01	25	W300	2 2 2 2 2	
5.307E-03	4.890E-01	25.35	U010	1 0 0 1 1	EFG
5.307E-03	4.890E-01	25.35	U013	1 0 0 0 0	EFG
3.255E-03	2.999E-01	30	F053	1 0 2 0 2	
6.183E-03	5.697E-01	30	G029	1 0 2 2 1	
5.067E-03	4.669E-01	30	M311	1 1 2 2 2	
1.409E-02	1.298E+00	30	S207	1 0 0 1 1	*sic*
5.557E-03	5.120E-01	34.53	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	34.53	U013	1 0 0 0 0	EFG
6.371E-03	5.870E-01	35	S203	1 1 2 1 2	
5.954E-03	5.486E-01	44.30	U010	1 0 0 1 1	EFG
5.819E-03	5.362E-01	44.30	U013	1 0 0 0 0	EFG
6.892E-03	6.350E-01	45	S203	1 1 2 1 2	
1.517E-02	1.398E+00	45	S207	1 0 0 1 1	*sic*
6.529E-03	6.015E-01	54.71	U013	1 0 0 0 0	EFG
1.500E-02	1.382E+00	55	H092	1 1 1 1 1	
6.380E-03	5.879E-01	55.79	U010	1 0 0 1 1	EFG
1.734E-02	1.597E+00	60	S207	1 0 0 1 1	*sic*
7.325E-03	6.749E-01	65.82	U013	1 0 0 0 0	EFG
2.171E-02	2.000E+00	150	J023	1 1 2 2 0	
7.597E-02	7.000E+00	200	J023	1 1 2 2 0	
3.039E-01	2.800E+01	250	J023	1 1 2 2 1	
1.411E+00	1.300E+02	300	J023	1 1 2 2 2	
5.589E-03	5.150E-01	ns	H123	0 0 0 0 0	
1.380E-01	1.272E+01	ns	H307	0 0 0 0 0	*sic*
5.611E-03	5.170E-01	ns	M175	0 0 2 1 2	
5.589E-03	5.150E-01	ns	M344	0 0 0 0 2	

1148. C_7H_8

1,6-Heptadiyne

RN: 2396-63-6 **MP** (°C)**:** –85
MW: 92.14 **BP** (°C)**:** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.791E-02	1.650E+00	25	M001	2 1 2 2 2	

1149. C_7H_8
Cycloheptatriene
1,3,5-Cycloheptatriene
Tropilidene
CHT
RN: 544-25-2 **MP** (°C)**:** –80
MW: 92.14 **BP** (°C)**:** 116.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.301E-03	5.806E-01	4.8	L007	2 2 1 2 2	
6.301E-03	5.806E-01	5.1	L007	2 1 1 1 2	
7.207E-03	6.641E-01	14.8	L007	2 2 1 2 2	
7.207E-03	6.641E-01	15.2	L007	2 1 1 1 2	
7.260E-03	6.690E-01	24.8	L007	2 2 1 2 2	
6.729E-03	6.200E-01	25	M001	2 1 2 2 2	
7.260E-03	6.690E-01	25.1	L007	2 1 1 1 2	
8.045E-03	7.413E-01	34.8	L007	2 2 1 2 2	
8.045E-03	7.413E-01	35.2	L007	2 1 1 1 2	
8.294E-03	7.642E-01	44.8	L007	2 2 1 2 2	
8.294E-03	7.642E-01	45.2	L007	2 1 1 1 2	

1150. $C_7H_8ClN_3O_4S_2$
Hydrochlorothiazide
Chlorozide
RN: 58-93-5 **MP** (°C)**:** 274
MW: 297.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.425E-03	7.220E-01	25	A076	1 0 1 1 2	
2.032E-03	6.050E-01	25	C437	0 0 0 0 0	Average
2.045E-03	6.090E-01	25	D091	1 0 0 0 2	pH 6.2
2.687E-03	8.000E-01	25	G051	1 0 1 1 0	
2.800E-03	8.337E-01	30	A089	2 0 1 1 0	EFG
2.800E-03	8.337E-01	30	A093	2 0 1 1 0	EFG
2.520E-03	7.503E-01	30	E049	2 0 2 2 2	
3.627E-03	1.080E+00	37	D091	1 0 0 0 2	pH 7.2
7.650E-03	2.278E+00	50	M335	1 0 2 1 2	pH 5
3.359E-03	1.000E+00	ns	K444	0 0 0 0 0	
1.982E-03	5.900E-01	rt	A095	0 0 0 0 0	

1151. $C_7H_8ClN_3O_4S_2$

Hydrochlorothiazide
3,4-Dihydro-6-chloro-7-sulfamoyl-1,2,4-benzothiadiazine-1,1-dioxide
3,4-Dihydrochlorothiazide
6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide
6-Chloro-3,4-dihydro-7-sulfamoyl-2H-1,2,4-benzothiadiazine-1,1-dioxide
Aldactazide

RN: 58-93-5 **MP** (°C)**:** 274
MW: 297.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.946E-01	22.5	B422	2 0 2 2 2	
2.351E-06	7.000E-04	25	A408	2 0 1 2 0	
2.115E-03	6.296E-01	25	S450	0 0 0 0 0	

1152. $C_7H_8FN_3O_3$

1-Ethylcarbamoyl-5-fluorouracil
1-Ethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
N-Ethyl-5-fluoro-3,4-dihydro-2,4-dioxo-1-pyrimidinecarboxamide

RN: 58471-47-9 **MP** (°C)**:** 190–196
MW: 201.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.457E-03	1.500E+00	22	B321	0 0 0 0 0	pH 4.0
7.457E-03	1.500E+00	22	B388	0 0 0 0 0	

1153. $C_7H_8FN_3O_3$

1-(*N,N*-Dimethylcarbamoyl)-5-fluorouracil
1-Dimethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

RN: 60908-29-4 **MP** (°C)**:** 226–227
MW: 201.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.983E-02	6.000E+00	22	B321	0 0 0 0 0	pH 4.0
2.983E-02	6.000E+00	22	B388	0 0 0 0 0	

1154. $C_7H_8N_2O_2$

3-Nitro-*o*-toluidine
3-Nitro-*o*-toluidin

RN: 603-83-8 **MP** (°C)**:** 92
MW: 152.15 **BP** (°C)**:** 305

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.807E-02	1.340E+01	100	F300	1 0 0 0 2	

1155. $C_7H_8N_2O_3$
5,5-Trimethylenebarbituric acid
6,8-Diazaspiro[3.5]nonane-5,7,9-trione
Cyclobutane-spirobarbiturate
RN: 6128-03-6 **MP** (°C)**:**
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.213E-02	3.721E+00	25	P350	0 0 0 0 0	intrinsic

1156. $C_7H_8N_2O_3$
1-Methoxy-2-amino-4-nitrobenzene
RN: 99-59-2 **MP** (°C)**:** 118
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-03	5.697E-01	rt	N015	0 0 2 2 2	

1157. $C_7H_8N_2O_3S$
5-Carboethoxy-2-thiouracil
Ethyl 2-thiouracil-5-carboxylate
RN: 38026-46-9 **MP** (°C)**:** 252
MW: 200.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.970E-03	1.596E+00	25	G016	1 2 1 2 2	intrinsic

1158. $C_7H_8N_2O_4$
Ethyl orotate
1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidine-carboxylic acid, ethyl ester
RN: 1747-53-1 **MP** (°C)**:**
MW: 184.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.867E+00	20	N019	0 0 0 0 0	

1159. $C_7H_8N_2S$
1-Phenyl-2-thiourea
Phenylthioharnstoff
RN: 103-85-5 **MP** (°C)**:** 149
MW: 152.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-02	2.600E+00	18	F300	1 0 0 0 1	
3.830E-01	5.830E+01	100	F300	1 0 0 0 2	

1160. $C_7H_8N_4O_2$
Theophylline
1,3-Dimethylxanthine
Aerolate
Bronkotabs
Bronchodid Duracap
Bronkodyl
RN: 58-55-9 **MP** (°C)**:** 272
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-02	5.964E+00	16	A072	1 0 1 0 1	
2.866E-02	5.164E+00	20	K052	1 1 1 1 2	
1.380E+00	2.486E+02	25	B443	0 0 0 0 0	
3.420E-02	6.162E+00	25	F009	2 2 2 2 0	EFG
3.675E-02	6.621E+00	25	L338	1 0 1 1 2	
4.089E-02	7.366E+00	25	M128	2 0 1 2 2	
4.083E-02	7.356E+00	25	M158	2 0 2 2 2	
3.580E-02	6.450E+00	25	N312	2 1 1 1 1	
4.607E-02	8.300E+00	25	P010	1 0 1 1 1	
4.607E-02	8.300E+00	25	P011	0 0 0 0 0	
4.440E-02	8.000E+00	25	P018	1 0 2 2 1	
4.440E-02	8.000E+00	25	P020	2 0 1 1 1	
4.607E-02	8.300E+00	25	P312	0 0 0 0 0	
4.500E-02	8.108E+00	30	B042	1 2 1 1 1	
4.500E-02	8.108E+00	30	G021	1 0 0 0 2	
4.100E-02	7.387E+00	30	H016	2 2 2 2 0	EFG
4.500E-02	8.108E+00	30	H020	1 0 0 0 1	
5.550E-02	1.000E+01	37	F076	2 0 2 2 0	
2.761E-02	4.975E+00	ns	J025	0 0 0 0 2	
5.550E-03	1.000E+00	ns	K444	0 0 0 0 0	
3.580E-02	6.450E+00	ns	N062	2 0 1 2 2	
2.054E-04	3.700E-02	rt	N015	0 0 2 2 1	*sic*

1161. $C_7H_8N_4O_2$
Theobromine
Theobromin
RN: 83-67-0 **MP** (°C)**:** 357
MW: 180.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.665E-03	3.000E-01	18	F300	1 0 0 0 0	
3.328E-03	5.996E-01	19	A072	1 0 1 0 0	
2.419E-03	4.358E-01	20	K052	1 1 1 1 2	
1.830E-03	3.297E-01	25	M158	2 0 2 2 2	
1.832E-03	3.300E-01	25	O302	1 0 0 1 0	
2.775E-03	5.000E-01	25	P010	1 0 1 1 1	
3.330E-03	6.000E-01	25	P011	0 0 0 0 0	
3.386E-03	6.100E-01	25	P018	1 0 2 2 1	

(*continued*)

1161. $C_7H_8N_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.108E-03	5.600E-01	25	P020	2 0 1 1 1	
3.000E-03	5.405E-01	30	B042	1 2 1 1 0	
~3.00E-03	~5.41E-01	30	H020	1 0 0 0 0	
3.830E-02	6.900E+00	100	F300	1 0 0 0 1	
2.774E-03	4.998E-01	c	D004	0 0 0 0 0	
3.676E-02	6.623E+00	h	D004	0 0 0 0 0	
>2.77E-03	>5.00E-01	ns	B404	0 2 1 1 0	

1162. C_7H_8O

p-Cresol
4-Cresol
p-Methylphenol

RN: 106-44-5 **MP** (°C)**:** 35.5
MW: 108.14 **BP** (°C)**:** 201.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.813E-01	1.961E+01	20	B031	1 0 2 2 1	
1.701E-01	1.840E+01	20	R087	0 0 0 0 0	0.15M NaCl
1.990E-01	2.152E+01	25	A021	1 2 1 1 0	
1.902E-01	2.057E+01	25	B019	1 0 1 2 0	
1.813E-01	1.961E+01	25	L022	1 0 0 0 0	
1.967E-01	2.127E+01	25	P004	0 0 0 0 0	
1.902E-01	2.057E+01	25	R041	0 0 0 0 0	
2.044E-01	2.210E+01	29.5	K119	1 0 0 0 2	
1.999E-01	2.162E+01	29.50	M098	1 2 0 1 2	
2.090E-01	2.260E+01	40	F300	1 0 0 0 2	
3.334E-01	3.605E+01	82.10	M098	1 2 0 1 2	

1163. C_7H_8O

Anisole
Methoxybenzene
Methyl phenyl ether
Phenyl methyl ether

RN: 100-66-3 **MP** (°C)**:** –37.3
MW: 108.14 **BP** (°C)**:** 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.295E-03	1.400E-01	25	A003	1 2 1 2 1	*sic*
9.609E-02	1.039E+01	25	B019	1 0 1 2 0	
1.000E-02	1.081E+00	25	D407	1 0 2 2 2	
1.400E-02	1.514E+00	25	M327	1 0 0 1 2	
1.418E-02	1.533E+00	25.04	V013	2 2 2 2 2	
9.617E-02	1.040E+01	26.70	L095	2 2 1 1 2	

1164. C_7H_8O

2-Cresol
2-Methylphenol
Phenol, 2-methyl-
o-Cresol
o-Methylphenol

RN: 95-48-7 **MP** (°C)**:** 31
MW: 108.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.519E-01	2.724E+01	20	B031	1 0 2 2 1	
2.276E-01	2.461E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.312E-01	2.500E+01	23	P332	0 0 0 0 0	
2.400E-01	2.595E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.127E-01	2.300E+01	25	B060	2 0 1 1 1	
2.400E-01	2.595E+01	25	B316	0 0 0 0 0	
2.300E-01	2.487E+01	25	F044	1 0 0 0 1	
2.423E-01	2.620E+01	25	F300	1 0 0 0 2	
2.569E-01	2.778E+01	25	L022	1 0 0 0 0	
2.999E-01	3.244E+01	25	P004	0 0 0 0 0	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
1.991E-01	2.153E+01	31	B092	2 1 1 1 2	
2.606E-01	2.818E+01	46.20	M098	1 2 0 1 1	
2.497E-01	2.700E+01	50	K119	1 0 0 0 2	
2.763E-01	2.988E+01	60	B092	2 1 1 1 2	
3.557E-01	3.846E+01	86.70	M098	1 2 0 1 1	
2.291E-01	2.477E+01	ns	R427	0 0 0 0 0	

1165. C_7H_8O

m-Cresol
3-Cresol
m-Methylphenol

RN: 108-39-4 **MP** (°C)**:** 11
MW: 108.14 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-01	1.147E+01	0	M041	1 1 0 0 2	
2.167E-01	2.344E+01	20	B031	1 2 2 2 1	
2.112E-01	2.284E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.149E-01	2.324E+01	20.3	L339	2 0 2 2 2	
1.420E-01	1.536E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.053E-01	2.220E+01	25	C060	1 2 1 1 2	
2.099E-01	2.270E+01	25	F300	1 0 0 0 2	
1.946E-01	2.105E+01	25	M041	1 1 0 0 2	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
2.292E-01	2.478E+01	40.0	L339	2 0 2 2 2	

(*continued*)

1165. C_7H_8O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-01	2.900E+01	46.2	K119	1 0 0 0 2	
2.326E-01	2.515E+01	50	M041	1 1 0 0 2	
2.431E-01	2.629E+01	50.80	M098	1 2 0 1 1	
2.712E-01	2.933E+01	58.4	L339	2 0 2 2 2	
2.693E-01	2.913E+01	60	B031	1 2 2 2 1	
3.331E-01	3.602E+01	77.2	L339	2 0 2 2 2	
3.213E-01	3.475E+01	78.70	M098	1 2 0 1 1	
3.982E-01	4.306E+01	92.20	M098	1 2 0 1 1	
4.387E-01	4.744E+01	98.1	L339	2 0 2 2 2	

1166. C_7H_8O

Benzyl alcohol
Benzylalkohol
Benzenemethanol
Phenylmethanol
Phenylcarbinol
α-Hydroxytoluene

RN: 100-51-6 **MP** (°C)**:** –15.2
MW: 108.14 **BP** (°C)**:** 204.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.606E-01	3.900E+01	17	F300	1 0 0 0 1	
3.488E-01	3.772E+01	20	H044	1 0 2 1 2	
3.520E-01	3.807E+01	20	S006	1 0 0 0 2	
3.967E-01	4.290E+01	25	B304	2 0 2 2 2	
3.540E-01	3.828E+01	25	H044	1 0 2 1 2	
4.260E-01	4.607E+01	25	L322	1 1 2 2 1	
3.616E-01	3.911E+01	30	H044	1 0 2 1 2	
3.646E-01	3.943E+01	35	H044	1 0 2 1 2	
3.676E-01	3.975E+01	40	H044	1 0 2 1 2	
3.724E-01	4.027E+01	45	H044	1 0 2 1 2	
3.722E-01	4.025E+01	50	H044	1 0 2 1 2	
3.868E-01	4.182E+01	55	H044	1 0 2 1 2	

1167. $C_7H_8O_2$

Salicyl alcohol
Salicylalkohol

RN: 90-01-7 **MP** (°C)**:** 86
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.075E-01	6.300E+01	22	F300	1 0 0 0 1	

1168. $C_7H_8O_2$
Guaiacol
o-Methoxyphenol
RN: 90-05-1 **MP** (°C)**:** 28
MW: 124.14 **BP** (°C)**:** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-01	1.870E+01	15	F300	1 0 0 0 2	
1.880E-01	2.334E+01	24.99	B353	0 0 0 0 0	
1.060E-02	1.316E+00	37	E028	1 0 1 1 2	*sic*
1.288E-03	1.599E-01	ns	R424	0 0 0 0 0	

1169. $C_7H_8O_2$
3-Methoxyphenol
Resorcinol monomethylether
p-Methoxyphenol
RN: 150-19-6 **MP** (°C)**:**
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-01	3.861E+01	25	B314	0 0 0 0 0	
3.110E-01	3.861E+01	30	B315	0 0 0 0 0	
4.000E-03	4.966E-01	37	E028	1 0 1 1 1	*sic*
4.966E-01	6.165E+01	ns	S460	0 0 0 0 0	

1170. $C_7H_8O_2$
p-Methoxyphenol
p-Hydroxyanisole
Hydroquinone monomethyl ether
4-Methoxyphenol
RN: 150-76-5 **MP** (°C)**:** 52.5
MW: 124.14 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-01	2.573E+01	20	R087	0 0 0 0 0	0.15M NaCl

1171. $C_7H_8O_2$

4,6-Dimethyl-1,2-pyrone
4,6-Dimethyl-α-pyrone
2,4-Dimethyl-α-pyrone
Mesitene lactone
4,6-Dimethyl-2-pyranone
4,6-Dimethyl-2H-pyran-2-one

RN: 675-09-2 **MP** (°C)**:** 49
MW: 124.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E+00	2.424E+02	59.7	W022	2 2 1 1 0	EFG
2.088E+00	2.593E+02	86.3	W022	2 2 1 1 0	EFG

1172. $C_7H_8O_3S$

p-Toluenesulfonic acid
4-Methylbenzenesulfonic acid
Methylbenzenesulfonic acid
Tosic acid
PTSA
Toluene-4-sulfonic acid

RN: 104-15-4 **MP** (°C)**:** 106.5
MW: 172.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E+00	4.993E+02	36.5	T023	1 2 2 1 2	
2.902E+00	4.997E+02	40.5	T023	1 2 2 1 2	
2.903E+00	4.999E+02	42.5	T023	1 2 2 1 2	

1173. $C_7H_8O_3S.H_2O$

p-Toluenesulfonic acid (monohydrate)

RN: 6192-52-5 **MP** (°C)**:** 104.5
MW: 190.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.008E+02	–6.5	T023	1 2 2 1 2	
2.120E+00	4.033E+02	–1.5	T023	1 2 2 1 2	
2.129E+00	4.050E+02	1.5	T023	1 2 2 1 2	
2.168E+00	4.125E+02	20.1	T023	1 2 2 1 2	
2.210E+00	4.203E+02	38.8	T023	1 2 2 1 2	
2.616E+00	4.975E+02	45.3	T023	1 2 2 1 2	
2.257E+00	4.293E+02	55.2	T023	1 2 2 1 2	
2.593E+00	4.933E+02	73.9	T023	1 2 2 1 2	
2.329E+00	4.431E+02	78.4	T023	1 2 2 1 2	
2.566E+00	4.882E+02	89.1	T023	1 2 2 1 2	
2.375E+00	4.517E+02	89.9	T023	1 2 2 1 2	

(*continued*)

1173. $C_7H_8O_3S.H_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.446E+00	4.652E+02	101.1	T023	1 2 2 1 2	
2.525E+00	4.802E+02	102.9	T023	1 2 2 1 2	
2.498E+00	4.751E+02	104.8	T023	1 2 2 1 2	

1174. $C_7H_8O_3S.2H_2O$

o-Toluenesulfonic acid (dihydrate)

RN: 68066-37-5 **MP** (°C)**:**

MW: 208.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E+00	3.577E+02	–25.0	T023	1 2 2 1 2	
1.773E+00	3.691E+02	–13.0	T023	1 2 2 1 2	
1.823E+00	3.795E+02	.8	T023	1 2 2 1 2	
1.891E+00	3.938E+02	16.8	T023	1 2 2 1 2	
1.954E+00	4.068E+02	31.2	T023	1 2 2 1 2	
2.264E+00	4.715E+02	48.2	T023	1 2 2 1 2	
2.055E+00	4.279E+02	50.0	T023	1 2 2 1 2	
2.243E+00	4.671E+02	54.0	T023	1 2 2 1 2	
2.090E+00	4.353E+02	56.0	T023	1 2 2 1 2	
2.207E+00	4.597E+02	60.4	T023	1 2 2 1 2	
2.148E+00	4.472E+02	61.2	T023	1 2 2 1 2	
2.179E+00	4.538E+02	62.0	T023	1 2 2 1 2	

1175. $C_7H_8O_3S.4H_2O$

p-Toluenesulfonic acid (tetrahydrate)

RN: 104-15-4 **MP** (°C)**:**

MW: 244.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E+00	3.473E+02	–27.0	T023	1 2 2 1 2	
1.437E+00	3.510E+02	–26.0	T023	1 2 2 1 2	
1.450E+00	3.543E+02	–18.5	T023	1 2 2 1 2	
1.527E+00	3.730E+02	–16.5	T023	1 2 2 1 2	
1.592E+00	3.888E+02	–10.5	T023	1 2 2 1 2	
1.613E+00	3.939E+02	–8.5	T023	1 2 2 1 2	
1.640E+00	4.005E+02	–7.0	T023	1 2 2 1 2	
1.576E+00	3.848E+02	–5.9	T023	1 2 2 1 2	
1.605E+00	3.921E+02	–3.4	T023	1 2 2 1 2	
1.622E+00	3.961E+02	–2.2	T023	1 2 2 1 2	
1.641E+00	4.008E+02	–1.0	T023	1 2 2 1 2	

1176. $C_7H_8O_7$
Methylenecitric acid
Methylen-citronensaeure
RN: 144-16-1 **MP** (°C)**:**
MW: 204.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-01	4.770E+01	20	F300	1 0 0 0 2	

1177. $C_7H_9ClN_2OS$
TO-2
5-Chloro-4-methyl-2-propionamide-thiazole
CMPT
RN: 13915-79-2 **MP** (°C)**:** 159
MW: 204.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.794E-04	1.800E-01	ns	M061	0 0 0 0 2	

1178. C_7H_9N
4-Ethylpyridine
4-Aethyl-pyridin
RN: 536-75-4 **MP** (°C)**:** –90.5
MW: 107.16 **BP** (°C)**:** 168.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.906E+00	4.186E+02	–19	C047	2 2 0 0 1	
2.495E+00	2.674E+02	182	C047	2 2 0 0 2	

1179. C_7H_9N
m-Toluidine
3-Toluidine
4-Methylaniline
p-Toluidine
p-Toluidin
RN: 106-49-0 **MP** (°C)**:** 43
MW: 107.16 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.066E-02	6.500E+00	15	F300	1 0 0 0 1	
6.026E-02	6.457E+00	20	B179	0 0 0 0 0	
3.890E-01	4.169E+01	20	B179	0 0 0 0 0	
1.403E-01	1.503E+01	20	C113	1 0 2 1 2	
6.200E-02	6.644E+00	20	H306	1 0 1 2 1	
6.119E-02	6.557E+00	20	T301	1 2 2 2 2	

1180. C_7H_9N
Methylaniline
N-Methylaniline
RN: 100-61-8 **MP** (°C)**:** –57
MW: 107.16 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.248E-02	5.624E+00	25	C113	1 0 2 1 2	

1181. C_7H_9N
3,4-Lutidine
3,4-Dimethylpyridine
RN: 583-58-4 **MP** (°C)**:** –12
MW: 107.16 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E+00	1.968E+02	–3.6	C047	2 2 0 0 2	
2.470E+00	2.647E+02	163	C047	2 2 0 0 1	
+2.29E+00	+2.45E+02	ns	S460	0 0 0 0 0	

1182. C_7H_9N
o-Toluidine
2-Toluidine
RN: 95-53-4 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.524E-01	1.633E+01	20	C113	1 0 2 1 2	
1.577E-01	1.690E+01	20	K119	1 0 0 0 2	
1.381E-01	1.480E+01	25	F300	1 0 0 0 2	

1183. C_7H_9N
3-Ethylpyridine
3-Aethyl-pyridin
β-Lutidine
RN: 536-78-7 **MP** (°C)**:**
MW: 107.16 **BP** (°C)**:** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	2.701E+02	196	C047	2 2 0 0 1	

1184. C_7H_9N
3,5-Lutidine
3,5-Dimethylpyridine
RN: 591-22-0 **MP** (°C)**:** –9
MW: 107.16 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	–12	C047	2 2 0 0 2	
2.520E+00	2.701E+02	192	C047	2 2 0 0 1	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1185. C_7H_9N
2,6-Lutidine
2,6-Dimethyl-pyridin
2,6-Dimethylpyridine
RN: 108-48-5 **MP** (°C)**:** –6
MW: 107.16 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E+00	2.308E+02	34	C047	2 2 0 0 1	
2.714E+00	2.908E+02	231	C047	2 2 0 0 1	
+2.82E+00	+3.02E+02	ns	S460	0 0 0 0 0	

1186. C_7H_9N
2,5-Lutidine
2,5-Dimethyl-pyridin
2,5-Dimethylpyridine
RN: 589-93-5 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.984E+00	2.126E+02	13.1	C047	2 2 0 0 1	
7.186E-01	7.700E+01	23	F300	1 0 0 0 1	
2.570E+00	2.754E+02	207	C047	2 2 0 0 1	

1187. C_7H_9N
2,4-Lutidine
2,4-Dimethyl-pyridin
2,4-Dimethylpyridine
RN: 108-47-4 **MP** (°C)**:** –60
MW: 107.16 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.961E+00	4.245E+02	23	J007	1 2 0 1 2	average of 2
1.896E+00	2.032E+02	23.4	C047	2 2 0 0 2	

(*continued*)

1187. C_7H_9N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	23.40	A009	1 2 1 1 2	LCST
1.287E+00	1.379E+02	24.40	A009	1 2 1 1 2	EFG, LCST
2.419E+00	2.593E+02	25	A009	1 2 1 1 2	EFG, LCST
3.316E+00	3.553E+02	27.2	J007	1 2 0 1 2	
8.484E-01	9.091E+01	30	A009	1 2 1 1 2	EFG, LCST
3.111E+00	3.333E+02	32.50	A009	1 2 1 1 2	EFG, LCST
4.497E+00	4.819E+02	35.0	J007	1 2 0 1 2	
2.902E+00	3.110E+02	39.0	J007	1 2 0 1 2	
6.105E-01	6.542E+01	40	A009	1 2 1 1 2	EFG, LCST
3.500E+00	3.750E+02	50	A009	1 2 1 1 2	EFG, LCST
2.545E+00	2.727E+02	53	J007	1 2 0 1 2	
4.548E+00	4.873E+02	54.3	J007	1 2 0 1 2	
3.777E+00	4.048E+02	62.50	A009	1 2 1 1 2	EFG, LCST
2.204E+00	2.362E+02	68.5	J007	1 2 0 1 2	
6.105E-01	6.542E+01	149	A009	1 2 1 1 2	EFG, UCST
3.794E+00	4.065E+02	165	A009	1 2 1 1 2	EFG, UCST
1.287E+00	1.379E+02	180	A009	1 2 1 1 2	EFG, UCST
3.500E+00	3.750E+02	180	A009	1 2 1 1 2	EFG, UCST
3.111E+00	3.333E+02	186	A009	1 2 1 1 2	EFG, UCST
1.896E+00	2.032E+02	187	A009	1 2 1 1 2	EFG, UCST
2.419E+00	2.593E+02	187	A009	1 2 1 1 2	EFG, UCST
2.520E+00	2.701E+02	189	A009	1 2 1 1 2	UCST
2.520E+00	2.701E+02	189	C047	2 2 0 0 1	

1188. C_7H_9N

2,3-Lutidine
2,3-Dimethylpyridine

RN: 583-61-9 **MP** (°C)**:** –15
MW: 107.16 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.926E+00	2.063E+02	16.5	C047	2 2 0 0 1	
2.594E+00	2.780E+02	193	C047	2 2 0 0 2	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1189. C_7H_9N

2-Ethylpyridine
α-Lutidine

RN: 100-71-0 **MP** (°C)**:**
MW: 107.16 **BP** (°C)**:** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E+00	2.537E+02	–5	C047	2 2 0 0 1	
2.760E+00	2.958E+02	231	C047	2 2 0 0 1	
+3.24E+00	+3.47E+02	ns	S460	0 0 0 0 0	

1190. C_7H_9NO
p-Anisidine
4-Methoxybenzenamine
p-Methoxyaniline
4-Methoxy-1-aminobenzene
p-Methoxyphenylamine
RN: 104-94-9 **MP** (°C)**:** 57
MW: 123.16 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-02	1.147E+01	20	T301	1 2 2 2 2	

1191. C_7H_9NO
p-Tolylhydroxylamine
p-Tolylhydroxylamin
RN: 623-10-9 **MP** (°C)**:**
MW: 123.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-02	1.000E+01	5	F300	1 0 0 0 1	
4.027E-01	4.960E+01	100	F300	1 0 0 0 2	

1192. C_7H_9NO
o-Anisidine
2-Anisidine
2-Methoxybenzenamine
o-Methoxyaniline
2-Methoxy-1-aminobenzene
o-Methoxyphenylamine
RN: 90-04-0 **MP** (°C)**:** 5
MW: 123.16 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-01	1.264E+01	25	B019	1 0 1 2 0	

1193. $C_7H_9NO_2$
1,2-Dimethyl-3-hydroxy-4-pyridone
DMHP
RN: 30652-11-0 **MP** (°C)**:** 271–273
MW: 139.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-01	1.572E+01	25	C340	0 0 0 0 0	pH 9.4

1194. $C_7H_9NO_2S$
p-Toluenesulfonamide
p-Methylbenzenesulfonamide
4-Methylbenzenesulfonamide
RN: 70-55-3 **MP** (°C)**:** 138
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.900E+00	9	F300	1 0 0 0 1	
1.180E-02	2.020E+00	15	K024	1 2 1 1 2	
1.843E-02	3.156E+00	25	H105	1 1 0 1 2	

1195. $C_7H_9NO_2S$
o-Toluenesulfonamide
o-Methylbenzenesulfonamide
RN: 88-19-7 **MP** (°C)**:** 156
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.840E-03	1.000E+00	9	F300	1 0 0 0 0	
1.860E-02	3.185E+00	15	K024	1 2 1 1 2	
9.485E-03	1.624E+00	25	H105	1 1 0 1 2	

1196. $C_7H_9NO_2S$
m-Toluenesulfonamide
m-Methylbenzenesulfonamide
RN: 1899-94-1 **MP** (°C)**:**
MW: 171.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E-02	2.996E+00	15	K024	1 2 1 1 2	
4.563E-02	7.812E+00	25	H105	1 1 0 1 2	

1197. $C_7H_9NO_3S$
4-Amino-3-methylbenzene sulfonic acid
4-Amino-toluol-sulfosaeure-(3)
RN: 98-33-9 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.671E-02	5.000E+00	20	F300	1 0 0 0 0	

1198. $C_7H_9NO_3S$
4-Amino-2-methylbenzene sulfonic acid
4-Amino-toluol-sulfosaeure-(2)
RN: 133-78-8 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.404E-02	4.500E+00	20	F300	1 0 0 0 1	

1199. $C_7H_9NO_3S$
2-Amino-5-methylbenzene sulfonic acid
2-Amino-toluol-sulfosaeure-(5)
RN: 88-44-8 **MP** (°C)**:** >300
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	3.200E+01	19	F300	1 0 0 0 1	

1200. $C_7H_9NO_3S$
p-Methoxybenzenesulfonamide
4-Methoxybenzenesulfonamide
RN: 1129-26-6 **MP** (°C)**:**
MW: 187.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	2.921E+00	15	K024	1 2 1 1 2	

1201. $C_7H_9N_3O$
4-Phenylsemicarbazide
Phenylsemicarbazide
RN: 537-47-3 **MP** (°C)**:** 123.5
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
	6.995E-01	15	D068	1 2 0 0 0	

1202. $C_7H_9N_3O_2S_2$
Sulfathiourea
p-Aminobenzenesulfonylthiourea
p-Aminophenylsulfonylthiourea
Badional
Baldinol
Fontamide
RN: 515-49-1 **MP** (°C)**:** 171.5
MW: 231.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.365E-03	5.470E-01	20	F073	1 2 2 2 2	

1203. $C_7H_9N_3O_3$
Orotic acid ethylamide
RN: 1011-82-1 **MP** (°C)**:** 263–265
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.553E+01	–4	N018	0 0 0 0 0	
3.240E-01	5.935E+01	16	N018	0 0 0 0 0	
3.980E-01	7.290E+01	25	N018	0 0 0 0 0	

1204. $C_7H_9N_3O_3S$
Sulfanilylurea
Sulfanilylharnstoff
RN: 547-44-4 **MP** (°C)**:** 146
MW: 215.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.333E+00	20	F073	1 2 2 2 2	
5.575E-03	1.200E+00	37	F300	1 0 0 0 1	
5.012E-02	1.079E+01	ns	R427	0 0 0 0 0	

1205. $C_7H_9N_3O_4$
Orotic acid ethanol amide
RN: **MP** (°C)**:** 217–218
MW: 199.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-01	3.585E+01	–4	N018	0 0 0 0 0	
3.460E-01	6.891E+01	16	N018	0 0 0 0 0	
4.470E-01	8.903E+01	25	N018	0 0 0 0 0	

1206. $C_7H_9O_3P$

Hydroxymethylphenylphosphinic acid

RN: 61451-78-3 **MP** (°C)**:** 138
MW: 172.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E+02	2.007E+04	0	W422	0 0 0 0 0	
9.900E+00	1.704E+03	34.29	W422	0 0 0 0 0	
2.060E+01	3.546E+03	44.30	W422	0 0 0 0 0	
4.240E+01	7.298E+03	54.41	W422	0 0 0 0 0	
9.660E+01	1.663E+04	64.99	W422	0 0 0 0 0	
1.662E+02	2.861E+04	73.42	W422	0 0 0 0 0	
2.474E+02	4.258E+04	79.6	W422	0 0 0 0 0	
3.120E+02	5.370E+04	83.95	W422	0 0 0 0 0	

1207. C_7H_{10}

1,3-Cycloheptadiene

RN: 4054-38-0 **MP** (°C)**:**
MW: 94.16 **BP** (°C)**:** 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-03	6.192E-01	ns	S460	0 0 0 0 0	

1208. $C_7H_{10}N_2OS$

Propylthiouracil
6-Propyl-2-thiouracil
Propycil

RN: 51-52-5 **MP** (°C)**:** 220.0
MW: 170.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.520E-03	1.110E+00	20	A091	1 0 0 0 0	
6.455E-03	1.099E+00	20	I310	0 0 0 0 0	
7.070E-03	1.204E+00	25	G016	1 2 1 2 2	intrinsic
5.816E-02	9.901E+00	100	I310	0 0 0 0 0	
5.874E-03	1.000E+00	ns	K444	0 0 0 0 0	

1209. $C_7H_{10}N_2O_2S$

p-Methylaminobenzenesulfonamide
4-Methylaminobenzenesulfonamide

RN: 16891-79-5 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	9.312E-01	15	K024	1 2 1 1 2	

1210. $C_7H_{10}N_2O_2S$
*N*1-Methylsulfanilamide
4-Amino-*N*-methylbenzenesulfonamide
N-Methyl-*p*-aminobenzenesulfonamide
N-Methyl-4-aminobenzenesulfonamide
RN: 1709-52-0 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-02	1.760E+01	37	K095	2 0 0 0 2	intrinsic

1211. $C_7H_{10}N_2O_2S$
Toluenesulfamide
Sulfamide, (4-methylphenyl)-
p-Tolylsulfamide
RN: 15853-38-0 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	5.624E+00	37	A028	1 0 2 1 2	intrinsic

1212. $C_7H_{10}N_2O_3$
Isopropylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-
Isopropylbarbiturate
RN: 7391-69-7 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.482E-02	5.925E+00	20	J030	1 2 2 2 2	
5.905E-02	1.005E+01	37	J030	1 2 2 2 2	

1213. $C_7H_{10}N_2O_3$
5-Ethyl-5-methylbarbituric acid
5-Methyl-5-ethylbarbituric acid
RN: 27653-63-0 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.010E-02	1.363E+01	25	M310	2 2 2 2 2	
5.912E-02	1.006E+01	25	P350	0 0 0 0 0	intrinsic

1214. $C_7H_{10}N_4O_2S$

Sulfanilylguanidine
Sulfaguanidine
Sulfaguanidin
Sulfanilguanidin

RN: 57-67-0 **MP** (°C)**:** 190
MW: 214.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.131E-03	8.850E-01	20	F073	1 2 2 2 2	
4.663E-03	9.990E-01	25	D041	1 0 0 0 0	
8.868E-03	1.900E+00	37	R045	1 2 1 1 2	
1.025E-02	2.195E+00	37.50	M142	1 2 0 0 2	
4.201E-01	9.000E+01	h	F300	0 0 0 0 0	

1215. $C_7H_{10}N_4O_3.H_2O$

Theopylline (monohydrate)
1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate

RN: 5967-84-0 **MP** (°C)**:** 269–272
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.823E-02	8.264E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

1216. $C_7H_{10}O_4S.H_2O$

o-Toluenesulfonic acid (monohydrate)
2-Methyl-benzenesulfonic acid (monohydrate)

RN: 88-20-0 **MP** (°C)**:**
MW: 208.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E+00	4.889E+02	32.5	T023	1 2 2 1 2	
2.335E+00	4.863E+02	38.6	T023	1 2 2 1 2	
2.318E+00	4.827E+02	45.7	T023	1 2 2 1 2	
2.266E+00	4.718E+02	48.5	T023	1 2 2 1 2	
2.302E+00	4.793E+02	48.6	T023	1 2 2 1 2	
2.273E+00	4.733E+02	49.0	T023	1 2 2 1 2	
2.289E+00	4.767E+02	49.6	T023	1 2 2 1 2	

1217. $C_7H_{10}O_5$
Shikimic acid
Shikimisaeure
RN: 138-59-0 **MP** (°C)**:** 190
MW: 174.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.613E-01	1.500E+02	21	F300	1 0 0 0 1	

1218. $C_7H_{10}O_5$
Mesoxalic acid diethyl ester
Mesooxalsaeure-diaethyl ester
RN: 609-09-6 **MP** (°C)**:** –30
MW: 174.15 **BP** (°C)**:** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.249E+00	5.658E+02	22	F300	1 0 0 0 2	
+3.25E+00	+5.66E+02	ns	S460	0 0 0 0 0	

1219. $C_7H_{11}NO_2$
Ethosuximide
Zarontin
2-Ethyl-2-methylsuccinimide
RN: 77-67-8 **MP** (°C)**:**
MW: 141.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E+00	1.900E+02	25	P061	0 0 0 0 0	pH 3-7.9
7.084E-01	1.000E+02	ns	K444	0 0 0 0 0	

1220. $C_7H_{11}N_3O_2$
Ipronidazole
1-Methyl-2-isopropyl-5-nitro-imidazole
RN: 14885-29-1 **MP** (°C)**:** 58–60
MW: 169.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-02	9.400E+00	20	D344	0 0 0 0 0	
5.550E-02	9.390E+00	20	D344	0 0 0 0 0	
5.446E-02	9.214E+00	20	D344	0 0 0 0 0	
5.560E-02	9.407E+00	20	D344	0 0 0 0 0	

1221. $C_7H_{11}N_3O_2$
1-Methyl-L-histidine
L-1-Methylhistidine
RN: 15507-76-3 **MP** (°C)**:** >254
MW: 169.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.851E-01	1.667E+02	25	D041	1 0 0 0 0	

1222. $C_7H_{11}N_7S$
Aziprotryne
2-Azido-4-isopropylamino-6-methylmercapto-*s*-triazine
C-7019
RN: 4658-28-0 **MP** (°C)**:** 95
MW: 225.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-04	5.500E-02	20	M161	1 0 0 0 1	
3.329E-04	7.500E-02	ns	M061	0 0 0 0 1	

1223. C_7H_{12}
1,6-Heptadiene
RN: 3070-53-9 **MP** (°C)**:** –129.0
MW: 96.17 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.575E-04	4.400E-02	25	M001	2 1 2 2 1	

1224. C_7H_{12}
1-Heptyne
1-*n*-Heptyne
Pentylacetylene
Amylacetylene
RN: 628-71-7 **MP** (°C)**:** –81
MW: 96.17 **BP** (°C)**:** 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.774E-04	9.400E-02	25	M001	2 1 2 2 2	

1225. C_7H_{12}
Cycloheptene
(1Z)-Cycloheptene
cis-Cycloheptene
RN: 628-92-2 **MP** (°C)**:** –56
MW: 96.17 **BP** (°C)**:** 114.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-04	6.600E-02	25	M001	2 1 2 2 1	

1226. C_7H_{12}
1-Methyl-1-cyclohexene
1-Methylcyclohexene
RN: 591-49-1 **MP** (°C)**:** –120
MW: 96.17 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-04	5.200E-02	25	M001	2 1 2 2 2	

1227. C_7H_{12}
2-Heptyne
1-Methyl-2-butylacetylene
Butyl(methyl)acetylene
RN: 1119-65-9 **MP** (°C)**:**
MW: 96.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	1.635E-01	25	H039	1 2 2 2 2	

1228. C_7H_{12}
2-Methyl-3-hexyne
1-Ethyl-2-isopropylacetylene
RN: 36566-80-0 **MP** (°C)**:**
MW: 96.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	1.731E-01	25	H039	1 2 2 2 2	

1229. $C_7H_{12}BrNO_4$

5-Bromo-2-propyl-5-nitro-1,3-dioxane
2-Propyl-5-bromo-5-nitro-1,3-dioxane
RN: 53983-01-0 **MP** (°C)**:** 73–75
MW: 254.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-03	2.799E-01	25	L013	1 0 2 1 2	

1230. $C_7H_{12}ClN_5$

Norazine
2-Chloro-4-methylamino-6-isopropylamino-*s*-triazine
RN: 3004-71-5 **MP** (°C)**:** 157–159
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	20	J033	0 0 0 0 0	
1.289E-03	2.600E-01	21	B192	0 0 0 0 2	

1231. $C_7H_{12}ClN_5$

Simazine
2-Chloro-4-ethylamino-6-ethylamino-*s*-triazine
2-Chloro-4,6-bis(ethylamino)-*s*-triazine
Primatol S
RN: 122-34-9 **MP** (°C)**:** 224
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.918E-06	2.000E-03	10	B185	0 0 0 0 0	
2.512E-05	5.065E-03	20	B179	0 0 0 0 0	
2.479E-05	5.000E-03	20	B185	0 0 0 0 0	
2.827E-05	5.700E-03	20	C048	2 2 2 2 1	
1.736E-05	3.500E-03	20	F311	1 2 2 2 1	
2.479E-05	5.000E-03	21	B192	0 0 0 0 0	
2.479E-05	5.000E-03	21	G099	2 0 0 1 0	
2.479E-05	5.000E-03	22	M061	1 0 0 0 0	
7.500E-05	1.512E-02	26	G001	1 0 1 1 1	
1.310E-04	2.642E-02	50	G001	1 0 1 1 2	
4.165E-04	8.400E-02	85	B185	0 0 0 0 0	
4.110E-04	8.288E-02	85	B200	1 0 0 0 2	
1.736E-05	3.500E-03	ns	C101	0 0 0 0 1	
2.479E-05	5.000E-03	ns	G041	0 0 0 0 0	
2.479E-05	5.000E-03	ns	H112	0 0 0 0 0	
2.479E-05	5.000E-03	ns	J033	0 0 0 0 0	
3.074E-05	6.200E-03	ns	V414	0 0 0 0 0	
2.479E-05	5.000E-03	rt	M161	0 0 0 0 0	

1232. $C_7H_{12}ClN_5$
2-Chloro-4-methyl amino-6-propyl amino-*s*-triazine
1,3,5-Triazine-2,4-diamine, 6-chloro-*N*-methyl-*N′*-propyl-*s*-Triazine, 2-chloro-4-methylamino-6-propylamino-
RN: 73383-40-1 **MP** (°C)**:**
MW: 201.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	21	G099	2 0 0 1 0	

1233. $C_7H_{12}N_2O_2$
5-Isobutylhydantoin
Hydantoin of DL-leucine
RN: 67337-73-9 **MP** (°C)**:** 208
MW: 156.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.937E+00	ns	M025	0 2 0 1 2	

1234. $C_7H_{12}N_4O_5$
Diglycine hydantoic acid
Carbamidoglycylglycine
RN: **MP** (°C)**:** 194
MW: 232.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-01	2.926E+01	25	M024	1 2 0 1 2	

1235. $C_7H_{12}N_4O_5$
Carbamidodiglycylglycine
Triglycine hydantoin acid
RN: **MP** (°C)**:** 204
MW: 232.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.460E-02	1.036E+01	25	M024	1 2 0 1 2	

1236. $C_7H_{12}O$
3-Methylcyclohexanone
m-Methylcyclohexanone
RN: 591-24-2 **MP** (°C)**:** –75
MW: 112.17 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.335E-02	1.498E+00	20	D052	1 1 0 0 0	
1.349E-02	1.513E+00	ns	S460	0 0 0 0 0	

1237. $C_7H_{12}O$
2-Methylcyclohexanone
Methyl anone
o-Methylcyohexanone
Methyl cyclohexanone
RN: 583-60-8 **MP** (°C)**:**
MW: 112.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-01	1.274E+01	23.50	O005	2 0 2 2 2	

1238. $C_7H_{12}O_2$
Hexahydrobenzoic acid
Cyclohexanecarboxylic acid
Cyclohexan-carbonsaeure
RN: 98-89-5 **MP** (°C)**:** 31
MW: 128.17 **BP** (°C)**:** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.006E+00	15	L006	1 0 0 0 2	
1.560E-02	2.000E+00	21	F300	1 0 0 0 0	

1239. $C_7H_{12}O_2$
Isobutyl propenoate
2-methylpropyl acrylate
2-Propenoic acid, 2-methylpropyl ester
Acrylic acid isobutyl ester
Isobutyl 2-propenoate
Isobutyl acrylate
RN: 106-63-8 **MP** (°C)**:**
MW: 128.17 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.166E-02	7.903E+00	ns	S460	0 0 0 0 0	

1240. $C_7H_{12}O_4$
Pimelic acid
Heptanedioc acid
RN: 111-16-0 **MP** (°C)**:** 105.7
MW: 160.17 **BP** (°C)**:** 272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-01	1.786E+01	5.99	A341	0 0 0 0 0	
1.151E-01	1.844E+01	7.99	A341	0 0 0 0 0	
1.334E-01	2.137E+01	10.99	A341	0 0 0 0 0	
1.523E-01	2.439E+01	13	D041	1 0 0 0 1	
1.498E-01	2.400E+01	13.50	F300	1 0 0 0 1	
3.122E-01	5.000E+01	15	M051	1 0 0 0 1	
2.236E-01	3.582E+01	15.99	A341	0 0 0 0 0	
2.527E-01	4.048E+01	17.99	A341	0 0 0 0 0	
3.006E-01	4.815E+01	19.99	A341	0 0 0 0 0	
2.973E-01	4.762E+01	20	D041	1 0 0 0 0	
3.122E-01	5.000E+01	20	L041	1 0 0 1 1	
2.953E-01	4.730E+01	20	M171	1 0 0 0 1	
3.000E-02	4.805E+00	20	S006	1 0 0 0 1	
3.332E+00	5.337E+02	21	B040	1 0 1 1 2	*sic*
3.846E-01	6.160E+01	23.99	A341	0 0 0 0 0	
3.938E-01	6.307E+01	24.99	A341	0 0 0 0 0	
4.660E-01	7.464E+01	28.99	A341	0 0 0 0 0	
5.072E-01	8.124E+01	30.99	A341	0 0 0 0 0	
5.690E-01	9.114E+01	33.99	A341	0 0 0 0 0	
6.545E-01	1.048E+02	36.99	A341	0 0 0 0 0	
8.886E-01	1.423E+02	39.99	A341	0 0 0 0 0	
1.527E+00	2.446E+02	42.99	A341	0 0 0 0 0	
1.824E+00	2.922E+02	44.99	A341	0 0 0 0 0	
2.135E+00	3.420E+02	47.49	A341	0 0 0 0 0	
2.551E+00	4.086E+02	49.99	A341	0 0 0 0 0	
3.460E+00	5.542E+02	54.82	A341	0 0 0 0 0	
3.915E+00	6.270E+02	59.99	A341	0 0 0 0 0	
4.365E+00	6.991E+02	64.49	A341	0 0 0 0 0	
4.649E+00	7.446E+02	68.99	A341	0 0 0 0 0	
3.937E-01	6.306E+01	rt	H431	0 0 0 0 0	

1241. $C_7H_{12}O_4$
Diethyl malonate
Malonic
Malonic ester
Propanedioic acid diethyl ester
Ethyl propanedioate
Ethyl methane dicarboxylate
RN: 105-53-3 **MP** (°C)**:** –50
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E+00	6.169E+02	25	H430	0 0 0 0 0	
1.450E-01	2.322E+01	37	E028	1 0 1 1 2	

1242. $C_7H_{12}O_4$
Ethyl α-acetoxypropionate
Ethyl 2-(acetyloxy)propanoate
Ethyl 2-acetoxypropionate
RN: 2985-28-6 **MP** (°C)**:**
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.104E-01	3.370E+01	25	R006	2 2 0 1 2	

1243. $C_7H_{12}O_4$
3-Methyladipic acid
3-Methylhexanedioic acid
RN: 3058-01-3 **MP** (°C)**:** 101
MW: 160.17 **BP** (°C)**:** 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.986E-01	6.385E+01	9.50	A031	1 2 2 2 2	
4.732E-01	7.579E+01	12.80	A031	1 2 2 2 2	
1.241E+00	1.987E+02	25.90	A031	1 2 2 2 2	
1.865E+00	2.987E+02	29.80	A031	1 2 2 2 2	
2.531E+00	4.055E+02	33.20	A031	1 2 2 2 2	
3.707E+00	5.938E+02	41.10	A031	1 2 2 2 2	
4.663E+00	7.468E+02	52.30	A031	1 2 2 2 2	
5.340E+00	8.553E+02	64.30	A031	1 2 2 2 2	

1244. $C_7H_{12}O_4$

n-Butylmalonic acid
Acide *n*-butylmalonique
RN: 534-59-8 **MP** (°C)**:** 102
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-01	1.160E+02	0	M051	1 0 0 0 2	
1.898E+00	3.040E+02	15	M051	1 0 0 0 2	
2.735E+00	4.380E+02	25	M051	1 0 0 0 2	
4.951E+00	7.930E+02	50	M051	1 0 0 0 2	

1245. $C_7H_{12}O_5$

Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 176.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.214E-02	1.623E+01	25	R007	0 0 0 0 0	

1246. $C_7H_{12}O_6$

Quinic acid
Chinasaeure
D-(–)-Quinic acid
1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid
RN: 77-95-2 **MP** (°C)**:** 162
MW: 192.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E+00	2.900E+02	9	F300	1 0 0 0 1	

1247. $C_7H_{13}BrN_2O_2$

Carbromal
Adalin
Bromodiethylacetylurea
N-(Aminocarbonyl)-2-bromo-2-ethylbutanamide
1-Bromo-ethyl-butyryl-urea
Bromodiethylacetylcarbamide
RN: 77-65-6 **MP** (°C)**:** 117
MW: 237.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E-03	5.000E-01	20	F300	1 0 0 0 0	

1248. $C_7H_{13}BrN_2O_2$

Bromo-pivalate ureide

RN: **MP** (°C)**:**

MW: 237.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-01	5.123E+01	ns	F057	0 2 2 2 1	

1249. $C_7H_{13}NO_2S$

2-Ethyl-2-methyl-4-thiazolidinecarboxylic acid

4-Thiazolidinecarboxylic acid, 2-ethyl-2-methyl-

Thiazolidine-4-carboxylic acid, 2-ethyl-2-methyl-

RN: 56595-20-1 **MP** (°C)**:**

MW: 175.25 **BP** (°C)**:** 327.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-01	4.557E+01	21	B414	1 0 0 1 1	very fast and extent decompostion, uncertain value

1250. $C_7H_{13}NO_2S$

2-Propylthiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2-propyl-

RN: 4165-34-8 **MP** (°C)**:**

MW: 175.25 **BP** (°C)**:** 346.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-02	1.490E+01	21	B414	1 0 0 1 1	partial decomposition

1251. $C_7H_{13}NO_2S_2$

2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-dithiolane

1,3-Dithiolane-4-methanol, 2,2-dimethyl-, carbamate

RN: 35801-62-8 **MP** (°C)**:**

MW: 207.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.244E+00	rt	B174	0 0 1 0 0	

1252. $C_7H_{13}NO_3$
N-Formylleucine
N-Formyl-DL-leucine
RN: 6113-61-7 **MP** (°C)**:**
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-01	2.945E+01	ns	M025	0 2 0 1 2	

1253. $C_7H_{13}NO_3S$
2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-oxathiolane
1,3-Oxathiolane-5-methanol, 2,2-dimethyl-, carbamate
RN: 78002-88-7 **MP** (°C)**:**
MW: 191.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	5.738E+00	rt	B174	0 0 1 0 0	

1254. $C_7H_{13}N_3O_3S$
Oxamyl
Vydate
Thioxamyl
N′,N′-Dimethyl-*N*-[(methylcarbamoyl)oxy]-1-thiooxamimidic acid methyl ester
N,N-Dimethyl-α-methylcarbamoyloxyimino-α-(methylthio)acetamide
DPX 1410
RN: 23135-22-0 **MP** (°C)**:** 109
MW: 219.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E+00	2.825E+02	20	B179	0 0 0 0 0	
1.277E+00	2.800E+02	25	M161	1 0 0 0 2	
9.977E-01	2.188E+02	ns	H308	0 0 0 0 1	

1255. $C_7H_{13}N_5O$
Hydroxysimazine
1,3,5-Triazin-2(1H)-one, 4,6-bis(ethylamino)-
2-Hydroxysimazine
4,6-bis(Ethylamino)-*s*-triazin-2-ol
G 30414
RN: 2599-11-3 **MP** (°C)**:**
MW: 183.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.748E-02	2	B193	1 1 0 0 1	

1256. C_7H_{14}
1-Heptene
1-*n*-Heptene
n-Hept-1-ene
RN: 592-76-7 **MP** (°C)**:** –119
MW: 98.19 **BP** (°C)**:** 93.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	1.817E-02	25	M342	1 0 1 1 2	

1257. C_7H_{14}
2-Heptene
RN: 592-77-8 **MP** (°C)**:**
MW: 98.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-04	1.500E-02	23.5	S171	2 1 2 2 2	
1.528E-04	1.500E-02	25	M001	2 1 2 2 1	

1258. C_7H_{14}
Cycloheptane
RN: 291-64-5 **MP** (°C)**:** –12
MW: 98.19 **BP** (°C)**:** 118.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-04	1.820E-02	20	M337	2 1 2 2 2	
3.055E-04	3.000E-02	25	M001	2 1 2 2 2	
2.760E-04	2.710E-02	30	G313	2 1 1 2 2	

1259. C_7H_{14}
Methylcyclohexane
Hexahydrotoluene
Methyl cyclohexane
RN: 108-87-2 **MP** (°C)**:** –126
MW: 98.19 **BP** (°C)**:** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-04	2.182E-02	2.34	S461	0 0 0 0 0	
2.000E-04	1.964E-02	9.99	S461	0 0 0 0 0	
1.711E-04	1.680E-02	20	B318	0 0 0 0 0	EFG
1.691E-04	1.660E-02	20	B356	0 0 0 0 0	
1.324E-04	1.300E-02	20	M337	2 1 2 2 2	
1.667E-04	1.636E-02	24.99	S461	0 0 0 0 0	
1.701E-04	1.670E-02	25	G313	2 1 1 2 2	
1.629E-04	1.600E-02	25	K119	1 0 0 0 2	

(*continued*)

1259. C_7H_{14} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	1.400E-02	25	M001	2 1 2 2 2	
1.426E-04	1.400E-02	25	M002	2 1 2 2 2	
1.629E-04	1.600E-02	25.0	P051	2 1 1 2 2	
1.629E-04	1.600E-02	25.00	P007	2 1 2 2 2	
1.644E-04	1.615E-02	26.1	M447	0 0 0 0 0	
1.375E-04	1.350E-02	28	B348	2 1 2 2 2	
1.833E-04	1.800E-02	40.1	P051	2 1 1 2 2	
1.833E-04	1.800E-02	40.10	P007	2 1 2 2 2	
1.925E-04	1.890E-02	55.7	P051	2 1 1 2 2	
1.925E-04	1.890E-02	55.70	P007	2 1 2 2 2	
2.800E-04	2.749E-02	70.5	M447	0 0 0 0 0	
3.442E-04	3.380E-02	99.1	P051	2 1 1 2 2	
3.442E-04	3.380E-02	99.10	P007	2 1 2 2 2	
5.589E-04	5.487E-02	100.5	M447	0 0 0 0 0	
8.097E-04	7.950E-02	120.0	P051	2 1 1 2 2	
8.097E-04	7.950E-02	120.00	P007	2 1 2 2 2	
1.355E-03	1.331E-01	131.0	M447	0 0 0 0 0	
1.416E-03	1.390E-01	137.3	P051	2 1 1 2 2	
1.416E-03	1.390E-01	137.30	P007	2 1 2 2 2	
2.485E-03	2.440E-01	149.5	P051	2 1 1 2 2	
2.485E-03	2.440E-01	149.50	P007	2 1 2 2 2	
2.349E-03	2.307E-01	151.4	M447	0 0 0 0 0	
1.426E-04	1.400E-02	ns	H123	0 0 0 0 0	

1260. $C_7H_{14}N_2O_2S$

Aldicarb
Temik
2-Methyl-2-(methylthio)propanal *O*-[(methylamino)carbonyl]oxime
UC 21149
N-Methylcarbamoyloxime,2-methyl-2-methylsulfenylpropionaldehyde
Methylcarbamic acid

RN: 116-06-3 **MP** (°C)**:** 99
MW: 190.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	6.017E+00	20	B179	0 0 0 0 0	
3.153E-02	6.000E+00	ns	H042	0 0 0 0 2	
3.135E-02	5.964E+00	ns	M061	0 0 0 0 0	
3.153E-02	6.000E+00	rt	M161	0 0 0 0 0	

1261. $C_7H_{14}N_2O_3$
ε-Aminocaproic hydantoic acid
ε-Uramidocaproic acid
RN: **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1262. $C_7H_{14}N_2O_3$
α-Aminocaproic hydantoic acid
α-Uramidocaproic acid
RN: **MP** (°C)**:** 169
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1263. $C_7H_{14}N_2O_4S_2$
Djenkoic acid
Djenkolsaeure
RN: 498-59-9 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-02	5.000E+00	100	F300	1 0 0 0 0	

1264. $C_7H_{14}N_6$
*N*2,*N*2,*N*4,*N*4-Tetramethylmelamine
Tetramethylmelamine
RN: 2827-47-6 **MP** (°C)**:** 227.0
MW: 182.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.052E-03	3.740E-01	25	C051	1 2 1 1 2	pH 7

1265. $C_7H_{14}O$
Cycloheptanol
RN: 502-41-0 **MP** (°C)**:**
MW: 114.19 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1266. $C_7H_{14}O$

Heptyl aldehyde
Heptanal
Oenanthaldehyd

RN: 111-71-7 **MP** (°C)**:** –43.3
MW: 114.19 **BP** (°C)**:** 152.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-02	3.100E+00	0	F300	1 0 0 0 1	
1.576E-02	1.800E+00	40	F300	1 0 0 0 1	

1267. $C_7H_{14}O$

4-Methyl-cyclohexanol

RN: 589-91-3 **MP** (°C)**:** –41
MW: 114.19 **BP** (°C)**:** 171–173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1268. $C_7H_{14}O$

Dipropyl ketone
4-Heptanone

RN: 123-19-3 **MP** (°C)**:** –32.6
MW: 114.19 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.430E-02	7.342E+00	0	G032	1 2 1 1 2	
4.660E-02	5.321E+00	10	G032	1 2 1 1 2	
3.750E-02	4.282E+00	20	D052	1 1 0 0 1	
2.793E-02	3.190E+00	25.50	O005	2 0 2 2 1	
3.350E-02	3.825E+00	30	G032	1 2 1 1 2	
2.880E-02	3.289E+00	50	G032	1 2 1 1 2	
2.720E-02	3.106E+00	75	G032	1 2 1 1 2	

1269. $C_7H_{14}O$

2-Heptanone
Heptan-2-one

RN: 110-43-0 **MP** (°C)**:** –31
MW: 114.19 **BP** (°C)**:** 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.489E-02	3.984E+00	20	D052	1 1 0 0 0	
3.836E-02	4.381E+00	20	G030	1 2 0 0 1	
3.800E-02	4.339E+00	20	M312	1 0 0 0 1	
3.750E-02	4.282E+00	25	G030	1 2 0 0 1	
1.675E-01	1.913E+01	25	P055	1 0 0 0 1	
3.570E-02	4.077E+00	25	W300	2 2 2 2 2	
3.489E-02	3.984E+00	30	G030	1 2 0 0 1	

1270. $C_7H_{14}O$
5-Methyl-2-hexanone
Methyl isoamyl ketone
Isopentyl methyl ketone
Methylhexanone
Methyl isoamyl ketone
MIAK
RN: 110-12-3 **MP** (°C)**:** –74
MW: 114.19 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.677E-02	5.341E+00	ns	S460	0 0 0 0 0	

1271. $C_7H_{14}O$
2,4-Dimethyl-3-pentanone
2,4-Dimethylpentanone-3
RN: 565-80-0 **MP** (°C)**:** –80
MW: 114.19 **BP** (°C)**:** 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.137E-02	5.865E+00	20	G030	1 2 0 0 1	
4.963E-02	5.668E+00	25	G030	1 2 0 0 1	
4.877E-02	5.569E+00	30	G030	1 2 0 0 1	
4.972E-02	5.677E+00	ns	J300	0 0 0 0 0	

1272. $C_7H_{14}O_2$
Heptoic acid
Heptanoic acid
n-Heptanoic acid
RN: 111-14-8 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-02	1.900E+00	0	B136	1 0 2 1 2	
1.843E-02	2.400E+00	15	F300	1 0 0 0 1	
1.847E-02	2.404E+00	15	L006	1 0 0 0 2	
1.721E-02	2.240E+00	20	B136	1 0 2 1 2	
1.870E-02	2.434E+00	20.0	R001	1 1 1 1 2	
2.161E-02	2.813E+00	25	H122	1 0 0 0 2	
2.082E-02	2.710E+00	30	B136	1 0 2 1 2	
2.076E-02	2.703E+00	30.0	R001	1 1 1 1 2	
2.389E-02	3.110E+00	45	B136	1 0 2 1 2	
2.381E-02	3.100E+00	45.0	R001	1 1 1 1 2	
2.711E-02	3.530E+00	60	B136	1 0 2 1 2	
2.702E-02	3.518E+00	60.0	R001	1 1 1 1 2	
1.457E-02	1.896E+00	.0	R001	1 1 1 1 2	

1273. $C_7H_{14}O_2$
Pentyl acetate
Amyl acetate
RN: 628-63-7 **MP** (°C)**:** –100
MW: 130.19 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-02	1.697E+00	20	D052	1 1 0 0 1	
1.290E-02	1.679E+00	20	S006	1 0 0 0 2	
1.329E-02	1.730E+00	25	K072	1 0 1 1 1	
1.329E-02	1.730E+00	25	M087	1 1 2 1 2	
3.060E-02	3.984E+00	30	R318	1 1 0 1 0	

1274. $C_7H_{14}O_2$
Isopropyl *N*-butyrate
Isopropyl butyrate
N-Butyric acid isopropyl ester
RN: 638-11-9 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-02	1.560E+00	ns	J300	0 0 0 0 0	

1275. $C_7H_{14}O_2$
3-Hydroxy-5-methyl-5-ethyltetrahydrofuran
3-Furanol, 5-ethyltetrahydro-5-methyl-
RN: 30010-08-3 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.983E-01	9.091E+01	rt	B066	0 2 0 0 1	

1276. $C_7H_{14}O_2$
Isoamyl acetate
Acetic acid isoamyl ester
Essigsaeureisoamyl ester
RN: 123-92-2 **MP** (°C)**:** –79
MW: 130.19 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	2.500E+00	15	F300	1 0 0 0 1	
1.222E-02	1.591E+00	20	E002	1 0 0 0 1	
1.227E-02	1.597E+00	23.50	O005	2 0 2 2 1	
1.533E-02	1.996E+00	25	L062	2 2 0 1 0	

1277. $C_7H_{14}O_2$
Methyl hexanoate
Methyl caproate
RN: 106-70-7 **MP** (°C)**:** –71.0
MW: 130.19 **BP** (°C)**:** 151.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E-02	1.325E+00	20	M337	2 1 2 2 2	

1278. $C_7H_{14}O_2$
Ethyl pentanoate
Ethyl *n*-valerate
Ethyl valerianate
RN: 539-82-2 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-02	2.226E+00	ns	S460	0 0 0 0 0	

1279. $C_7H_{14}O_2$
n-Butyl propionate
Butyl propionate
RN: 590-01-2 **MP** (°C)**:** –89
MW: 130.19 **BP** (°C)**:** 146.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-02	1.498E+00	20	D052	1 1 0 0 0	
9.500E-03	1.237E+00	25	K012	1 0 0 0 1	
1.514E-02	1.970E+00	ns	S460	0 0 0 0 0	

1280. $C_7H_{14}O_2$
Propyl butyrate
Buttersaeure-propyl ester
n-Propyl *n*-butyrate
RN: 105-66-8 **MP** (°C)**:** –95
MW: 130.19 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.614E+00	17	F001	1 0 1 0 2	
1.244E-02	1.620E+00	17	F300	1 0 0 0 2	
1.200E-02	1.562E+00	17	S006	1 0 0 0 1	

1281. $C_7H_{14}O_2$
sec-Amyl acetate
2-Pentyl acetate
1-Methylbutyl acetate
RN: 53496-15-4 **MP** (°C)**:**
MW: 130.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-02	1.896E+00	20	D052	1 1 0 0 0	

1282. $C_7H_{14}O_3$
n-Ethyl β-ethoxypropionate
Ethyl β-ethoxypropionate
RN: 763-69-9 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:** 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-01	5.258E+01	25	D002	1 2 1 1 2	
3.566E-01	5.213E+01	25	R034	0 0 0 0 1	

1283. $C_7H_{14}O_3$
Butyl lactate
Butyl α-hydroxypropionate
2-Propanoic acid
Lactic acid butyl ester
Butyl 2-hydroxypropanoate
RN: 138-22-7 **MP** (°C)**:** –28
MW: 146.19 **BP** (°C)**:** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.631E-01	3.846E+01	20	D052	1 1 0 0 1	
2.982E-01	4.360E+01	25	R006	2 2 0 1 2	

1284. $C_7H_{14}O_3$
n-Propyl β-methoxypropionate
Propionic acid, 3-methoxy-, propyl ester
RN: 5349-56-4 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E-01	3.101E+01	25	R034	0 0 0 0 1	

1285. $C_7H_{14}O_3$
Methyl β-*n*-propoxypropionate
Propanoic acid, 3-propoxy-, methyl ester
RN: 14144-39-9 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.249E-01	3.288E+01	25	R034	0 0 0 0 1	

1286. $C_7H_{14}O_3$
3-Methoxy butyl acetate
3-Methoxy-1-butanol acetate
Methyl-1,3-butylene glycol acetate
3-Methoxybutyl acetate
Butoxyl
Butoxyl (3-methoxy-*N*-butyl acetate)
RN: 4435-53-4 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.151E-01	6.068E+01	20	D052	1 1 0 0 2	

1287. $C_7H_{14}O_6$
β-Methyl-D-glucoside
β-Methyl-D-glucosid
RN: 709-50-2 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.892E+00	3.674E+02	17	F300	1 0 0 0 2	

1288. $C_7H_{14}O_6$
α-D-Methylglucoside
α-Methyl-D-glucoside
α-Methyl-D-glucosid
RN: 97-30-3 **MP** (°C)**:** 168
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E+00	3.868E+02	17	F300	1 0 0 0 2	
2.543E+00	4.938E+02	17.8	W013	1 2 1 1 2	
2.637E+00	5.120E+02	22.5	W013	1 2 1 1 2	
2.657E+00	5.159E+02	25.5	W013	1 2 1 1 2	
2.696E+00	5.236E+02	26.6	W013	1 2 1 1 2	
2.699E+00	5.241E+02	27.3	W013	1 2 1 1 2	

(*continued*)

1288. $C_7H_{14}O_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.751E+00	5.342E+02	31.8	W013	1 2 1 1 2	
2.806E+00	5.448E+02	33.9	W013	1 2 1 1 2	
2.849E+00	5.533E+02	37.2	W013	1 2 1 1 2	
2.951E+00	5.731E+02	43.2	W013	1 2 1 1 2	
3.060E+00	5.942E+02	49.0	W013	1 2 1 1 2	
3.078E+00	5.978E+02	49.6	W013	1 2 1 1 2	
3.131E+00	6.079E+02	51.8	W013	1 2 1 1 2	
3.166E+00	6.148E+02	54.4	W013	1 2 1 1 2	
3.213E+00	6.240E+02	57.3	W013	1 2 1 1 2	
3.297E+00	6.402E+02	60.6	W013	1 2 1 1 2	
3.332E+00	6.471E+02	62.7	W013	1 2 1 1 2	
3.360E+00	6.525E+02	64.2	W013	1 2 1 1 2	
3.403E+00	6.608E+02	66.2	W013	1 2 1 1 2	
3.435E+00	6.670E+02	67.8	W013	1 2 1 1 2	
3.542E+00	6.878E+02	73.2	W013	1 2 1 1 2	
3.651E+00	7.090E+02	78.0	W013	1 2 1 1 2	

1289. $C_7H_{14}O_6$

α-Methyl-D-mannoside
α-Methyl-D-mannosid
RN: 617-04-9 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.976E+02	17	F300	1 0 0 0 2	

1290. $C_7H_{14}O_7$

D-Mannoheptose
D-Sedoheptose
RN: 7634-39-1 **MP** (°C)**:**
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.76E-01	>1.00E+02	20	F300	1 0 0 0 0	

1291. $C_7H_{14}O_7$

D-α-Glucoheptose
Gluco-heptose
RN: 62475-58-5 **MP** (°C)**:**
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	8.676E+01	20	D041	1 0 0 0 1	

1292. $C_7H_{15}Br$
1-Bromoheptane
Heptyl bromide
RN: 629-04-9 **MP** (°C)**:** –56.1
MW: 179.11 **BP** (°C)**:** 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-05	6.645E-03	25	M342	1 0 1 1 2	

1293. $C_7H_{15}Cl$
1-Chloroheptane
Heptyl chloride
RN: 629-06-1 **MP** (°C)**:** –69.5
MW: 134.65 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-04	1.360E-02	25	M342	1 0 1 1 2	

1294. $C_7H_{15}Cl_2N_2O_2P$
Cyclophosphamide
Cyclophosphoramide
2-(bis(2-Chloroethyl)-amino)tetrahydro-2H-1,3,2-oxazaphosphorine 2-oxide
Cycloblastin
Sendoxan
Claphene
RN: 50-18-0 **MP** (°C)**:**
MW: 261.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.532E-01	4.000E+01	ns	K444	0 0 0 0 0	

1295. $C_7H_{15}I$
1-Iodoheptane
Heptyl iodide
RN: 4282-40-0 **MP** (°C)**:** –48.2
MW: 226.10 **BP** (°C)**:** 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-05	3.505E-03	25	M342	1 0 1 1 2	

1296. $C_7H_{15}NO_2$
Isobutyl urethane
Isobutylurethan
RN: 539-89-9 **MP** (°C)**:**
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	2.482E+01	15.5	F001	1 0 1 2 2	

1297. $C_7H_{15}NO_2$
n-Hexyl carbamate
Hexyl carbamate
RN: 2114-20-7 **MP** (°C)**:** 62
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	1.742E+00	37	H006	1 2 2 1 1	

1298. $C_7H_{15}NO_2$
tert-Hexyl carbamate
3,3-Dimethyl-1-butanol carbamate
RN: 3124-38-7 **MP** (°C)**:**
MW: 145.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.937E+00	37	H006	1 2 2 1 1	

1299. C_7H_{16}
3,3-Dimethylpentane
3,3-Dwumetylopentan
RN: 562-49-2 **MP** (°C)**:** –135
MW: 100.21 **BP** (°C)**:** 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.928E-05	5.940E-03	25	K119	1 0 0 0 2	
5.908E-05	5.920E-03	25.0	P051	2 1 1 2 2	
5.908E-05	5.920E-03	25.00	P007	2 1 2 2 2	
6.766E-05	6.780E-03	40.1	P051	2 1 1 2 2	
6.766E-05	6.780E-03	40.10	P007	2 1 2 2 2	
8.153E-05	8.170E-03	55.7	P051	2 1 1 2 2	
8.153E-05	8.170E-03	55.70	P007	2 1 2 2 2	
1.028E-04	1.030E-02	69.7	P051	2 1 1 2 2	
1.028E-04	1.030E-02	69.70	P007	2 1 2 2 2	
1.577E-04	1.580E-02	99.1	P051	2 1 1 2 2	

(*continued*)

1299. C_7H_{16} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-04	1.580E-02	99.10	P007	2 1 2 2 2	
2.724E-04	2.730E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	118.00	P007	2 1 2 2 2	
6.716E-04	6.730E-02	120.4	P051	2 1 1 2 2	
6.716E-04	6.730E-02	120.40	P007	2 1 2 2 2	
8.592E-04	8.610E-02	150.4	P051	2 1 1 2 2	
8.592E-04	8.610E-02	150.40	P007	2 1 2 2 2	

1300. C_7H_{16}
3-Methylhexane
3-Metyloheksan
RN: 589-34-4 **MP** (°C)**:** –119
MW: 100.21 **BP** (°C)**:** 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.229E-05	5.240E-03	0	P003	2 2 2 2 2	
1.048E-04	1.050E-02	23	C332	0 0 0 0 0	
2.635E-05	2.640E-03	25	K119	1 0 0 0 2	
4.940E-05	4.950E-03	25	P003	2 2 2 2 2	
2.635E-05	2.640E-03	25	P051	2 1 1 2 2	
2.635E-05	2.640E-03	25.00	P007	2 1 2 2 2	

1301. C_7H_{16}
2,4-Dimethylpentane
2,4-Dwumetylopentan
RN: 108-08-7 **MP** (°C)**:** –123
MW: 100.21 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.487E-05	6.500E-03	0	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	K119	1 0 0 0 2	
4.052E-05	4.060E-03	25	M001	2 1 2 2 2	
3.613E-05	3.620E-03	25	M002	2 1 2 2 2	
5.489E-05	5.500E-03	25	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	P051	2 1 1 2 2	
4.401E-05	4.410E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1302. C_7H_{16}
2,3-Dimethylpentane
2,3-Dwumetylopentan
RN: 565-59-3 **MP** (°C)**:** <25
MW: 100.21 **BP** (°C)**:** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.239E-05	5.250E-03	25	K119	1 0 0 0 2	
5.239E-05	5.250E-03	25	P051	2 1 1 2 2	
5.239E-05	5.250E-03	25.00	P007	2 1 2 2 2	

1303. C_7H_{16}
2-Methylhexane
2-Metyloheksan
RN: 591-76-4 **MP** (°C)**:** –118
MW: 100.21 **BP** (°C)**:** 90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	1.400E-02	23	C332	0 0 0 0 0	
2.535E-05	2.540E-03	25	K119	1 0 0 0 2	
2.535E-05	2.540E-03	25	P051	2 1 1 2 2	
2.535E-05	2.540E-03	25.00	P007	2 1 2 2 2	

1304. C_7H_{16}
2,2-Dimethylpentane
2,2-Dwumetylopentan
RN: 590-35-2 **MP** (°C)**:** –123
MW: 100.21 **BP** (°C)**:** 79.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.391E-05	4.400E-03	25	K119	1 0 0 0 2	
4.391E-05	4.400E-03	25	P051	2 1 1 2 2	
4.391E-05	4.400E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1305. C_7H_{16}
Heptane
n-Heptane
RN: 142-82-5 **MP** (°C)**:** –90.7
MW: 100.21 **BP** (°C)**:** 98.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.381E-05	4.390E-03	0	P003	2 2 2 2 2	
8.333E-05	8.350E-03	2.34	S461	0 0 0 0 0	

(*continued*)

1305. C_7H_{16} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-05	1.954E-03	4.3	N004	1 1 2 2 2	
1.667E-05	1.670E-03	9.99	S461	0 0 0 0 0	
2.017E-05	2.021E-03	13.5	N004	1 1 2 2 2	
4.990E-04	5.000E-02	15	F300	1 0 0 0 1	
5.200E-04	5.211E-02	15.50	F001	1 0 1 0 2	
1.497E-04	1.500E-02	16	D047	1 0 0 1 0	
2.694E-05	2.700E-03	20	M337	2 1 2 2 1	
1.111E-05	1.113E-03	24.99	S461	0 0 0 0 0	
3.990E-03	3.998E-01	25	G323	2 2 2 2 0	
4.990E-04	5.000E-02	25	K072	1 0 1 1 1	
2.235E-05	2.240E-03	25	K119	1 0 0 0 2	
2.924E-05	2.930E-03	25	M001	2 1 2 2 2	
2.924E-05	2.930E-03	25	M002	2 1 2 2 2	
4.990E-04	5.000E-02	25	M087	1 1 2 1 0	
3.050E-05	3.056E-03	25	M342	1 0 1 1 2	
3.363E-05	3.370E-03	25	P003	2 2 2 2 2	
4.989E-04	5.000E-02	25	S012	2 0 2 2 0	
2.656E-05	2.661E-03	25.0	N004	1 1 2 2 2	
2.235E-05	2.240E-03	25.0	P051	2 1 1 2 2	
2.235E-05	2.240E-03	25.00	P007	2 1 2 2 2	
2.261E-05	2.266E-03	35.0	N004	1 1 2 2 2	
2.625E-05	2.630E-03	40.1	P051	2 1 1 2 2	
2.400E-05	2.405E-03	45.0	N004	1 1 2 2 2	
8.973E-03	8.992E-01	50	G323	2 2 2 2 0	
3.104E-05	3.110E-03	55.7	P051	2 1 1 2 2	
3.104E-05	3.110E-03	55.70	P007	2 1 2 2 2	
5.589E-05	5.600E-03	99.1	P051	2 1 1 2 2	
5.589E-05	5.600E-03	99.10	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.6	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.60	P007	2 1 2 2 2	
4.361E-04	4.370E-02	150.4	P051	2 1 1 2 2	
4.361E-04	4.370E-02	150.40	P007	2 1 2 2 2	
3.692E-05	3.700E-03	ns	B151	0 2 1 1 1	
7.000E-04	7.014E-02	ns	H012	0 2 2 0 0	

1306. $C_7H_{16}O$

3-Heptanol
(±)-3-Heptanol
3-Hydroxyheptane
1-Ethyl-1-pentanol

RN: 589-82-2 **MP** (°C)**:** –70
MW: 116.20 **BP** (°C)**:** 156.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-02	4.764E+00	20	H330	0 0 0 0 0	
3.428E-02	3.984E+00	25	C093	2 1 1 1 0	

1307. $C_7H_{16}O$
2-Heptanol
2-Hydroxyheptane
Amylmethylcarbinol
RN: 543-49-7 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 159.00

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.532E-02	6.428E+00	0	S307	1 1 0 2 2	
3.966E-02	4.609E+00	10.2	S307	1 1 0 2 2	
3.633E-02	4.222E+00	19.5	S307	1 1 0 2 2	
3.001E-02	3.488E+00	30.7	S307	1 1 0 2 2	
2.813E-02	3.269E+00	40.0	S307	1 1 0 2 2	
2.514E-02	2.921E+00	50.0	S307	1 1 0 2 2	
2.471E-02	2.872E+00	60.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	70.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	80.0	S307	1 1 0 2 2	
2.942E-02	3.418E+00	90.2	S307	1 1 0 2 2	

1308. $C_7H_{16}O$
3-Methyl-3-hexanol
3-Methylhexanol-3
RN: 597-96-6 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.146E-01	1.332E+01	20	G006	1 2 1 1 2	
1.012E-01	1.176E+01	25	G006	1 2 1 1 2	
9.110E-02	1.059E+01	30	G006	1 2 1 1 2	

1309. $C_7H_{16}O$
3-Ethyl-3-pentanol
3-Ethyl-pentanol-3
Triethyl carbinol
RN: 597-49-9 **MP** (°C)**:** –12
MW: 116.20 **BP** (°C)**:** 141.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-01	1.874E+01	20	G006	1 2 1 1 2	
1.422E-01	1.652E+01	25	G006	1 2 1 1 2	
1.272E-01	1.478E+01	30	G006	1 2 1 1 2	
1.071E-01	1.244E+01	40	G006	1 2 1 1 2	

1310. $C_7H_{16}O$

2-Methyl-2-hexanol
2-Methylhexanol-2
RN: 625-23-0 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.195E-02	1.068E+01	20	G006	1 2 1 1 2	
8.267E-02	9.607E+00	25	G006	1 2 1 1 1	
7.422E-02	8.625E+00	30	G006	1 2 1 1 1	

1311. $C_7H_{16}O$

2,4-Dimethyl-3-pentanol
2,4-Dimethylpentanol-3
Diisopropyl carbinol
RN: 600-36-2 **MP** (°C)**:** –70
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.172E+01	0	S307	1 1 0 2 2	
8.942E-02	1.039E+01	10.0	S307	1 1 0 2 2	
6.660E-02	7.740E+00	20	G006	1 2 1 1 1	
6.067E-02	7.050E+00	20.2	S307	1 1 0 2 2	
1.935E-01	2.248E+01	24.50	O005	2 0 2 2 1	
5.982E-02	6.951E+00	25	G006	1 2 1 1 1	
5.727E-02	6.655E+00	30	G006	1 2 1 1 1	
5.489E-02	6.379E+00	30.6	S307	1 1 0 2 2	
4.562E-02	5.302E+00	39.5	S307	1 1 0 2 2	
4.332E-02	5.035E+00	49.7	S307	1 1 0 2 2	
3.992E-02	4.638E+00	60.3	S307	1 1 0 2 2	
3.778E-02	4.391E+00	70.2	S307	1 1 0 2 2	
3.667E-02	4.262E+00	80.2	S307	1 1 0 2 2	
3.855E-02	4.480E+00	90.6	S307	1 1 0 2 2	

1312. $C_7H_{16}O$

2,4-Dimethyl-2-pentanol
2,4-Dimethylpentanol-2
RN: 625-06-9 **MP** (°C)**:** <–20
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-01	1.478E+01	20	G006	1 2 1 1 2	
1.138E-01	1.322E+01	25	G006	1 2 1 1 2	
1.037E-01	1.205E+01	30	G006	1 2 1 1 2	

1313. $C_7H_{16}O$

2,3-Dimethyl-2-pentanol
2,3-Dimethylpentanol-2
RN: 4911-70-0 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-01	1.662E+01	20	G006	1 2 1 1 2	
1.305E-01	1.517E+01	25	G006	1 2 1 1 2	
1.188E-01	1.381E+01	30	G006	1 2 1 1 2	

1314. $C_7H_{16}O$

2,3,3-Trimethyl-2-butanol
Dimethyl-*tert*-butylcarbinol
1,1,2,2-Tetramethylpropanol
1,1,2,2-Tetramethylpropyl alcohol
RN: 594-83-2 **MP** (°C)**:** 17
MW: 116.20 **BP** (°C)**:** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.852E-01	2.153E+01	40	G006	1 2 1 1 2	

1315. $C_7H_{16}O$

2,2-Dimethyl-3-pentanol
2,2-Dimethylpentanol-3
RN: 3970-62-5 **MP** (°C)**:** –5
MW: 116.20 **BP** (°C)**:** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.507E-02	8.723E+00	20	G006	1 2 1 1 1	
6.999E-02	8.133E+00	25	G006	1 2 1 1 1	
6.745E-02	7.838E+00	30	G006	1 2 1 1 1	

1316. $C_7H_{16}O$

1-Heptanol
1-Hydroxyheptane
Heptan-1-ol
Heptanol-(1)
n-Heptyl alcohol
RN: 111-70-6 **MP** (°C)**:** –34.6
MW: 116.20 **BP** (°C)**:** 175.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.916E-02	3.388E+00	0	E029	1 2 0 1 1	
2.026E-02	2.354E+00	0	S307	1 1 0 2 2	
1.897E-02	2.205E+00	6.04	H110	2 2 2 2 2	

(*continued*)

1316. $C_7H_{16}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-02	2.593E+00	10	E029	1 2 0 1 1	
1.739E-02	2.020E+00	10.24	H110	2 2 2 2 2	
2.172E-02	2.524E+00	10.5	S307	1 1 0 2 2	
1.720E-02	1.999E+00	10.54	H110	2 2 2 2 2	
1.067E-02	1.240E+00	11.4	N042	1 0 2 1 1	
1.608E-02	1.869E+00	15.04	H110	2 2 2 2 2	
1.544E-02	1.795E+00	17.94	H110	2 2 2 2 2	
8.000E-03	9.296E-01	18	F001	1 0 1 0 2	
8.605E-03	1.000E+00	18	F300	1 0 0 0 1	
1.478E-02	1.717E+00	20	A015	1 2 1 1 2	
1.718E-02	1.996E+00	20	E029	1 2 0 1 1	
1.450E-02	1.685E+00	20	H330	0 0 0 0 0	
1.507E-02	1.751E+00	20.04	H110	2 2 2 2 2	
1.581E-02	1.837E+00	20.2	S307	1 1 0 2 2	
1.476E-02	1.716E+00	21.94	H110	2 2 2 2 2	
1.450E-02	1.685E+00	23.94	H110	2 2 2 2 2	
1.443E-02	1.677E+00	24.94	H110	2 2 2 2 2	
1.546E-02	1.797E+00	25	B038	1 2 1 1 2	
1.000E+00	1.162E+02	25	F044	1 0 0 0 0	EFG
1.460E-02	1.697E+00	25	K025	2 1 1 1 1	
1.434E-02	1.666E+00	25.04	H110	2 2 2 2 2	
1.423E-02	1.653E+00	26.04	H110	2 2 2 2 2	
1.411E-02	1.640E+00	28.04	H110	2 2 2 2 2	
1.375E-02	1.597E+00	30	E029	1 2 0 1 1	
1.397E-02	1.624E+00	30.14	H110	2 2 2 2 2	
1.399E-02	1.626E+00	30.14	H110	2 2 2 2 2	
1.323E-02	1.538E+00	30.6	S307	1 1 0 2 2	
1.386E-02	1.611E+00	32.94	H110	2 2 2 2 2	
1.426E-02	1.657E+00	39.8	S307	1 1 0 2 2	
1.117E-02	1.298E+00	40	E029	1 2 0 1 1	
9.456E-03	1.099E+00	50	E029	1 2 0 1 1	
1.392E-02	1.617E+00	50.1	S307	1 1 0 2 2	
9.456E-03	1.099E+00	60	E029	1 2 0 1 1	
1.529E-02	1.777E+00	60.0	S307	1 1 0 2 2	
1.289E-02	1.498E+00	70	E029	1 2 0 1 1	
1.080E-02	1.255E+00	70	F001	1 0 1 0 2	
1.752E-02	2.036E+00	70.1	S307	1 1 0 2 2	
1.632E-02	1.896E+00	80	E029	1 2 0 1 1	
1.460E-02	1.697E+00	80	F001	1 0 1 0 2	
1.863E-02	2.165E+00	80.1	S307	1 1 0 2 2	
1.975E-02	2.295E+00	90	E029	1 2 0 1 1	
1.940E-02	2.254E+00	90	F001	1 0 1 0 2	
2.086E-02	2.424E+00	90.5	S307	1 1 0 2 2	
2.488E-02	2.892E+00	100	E029	1 2 0 1 1	
2.460E-02	2.859E+00	100	F001	1 0 1 0 2	
2.582E-02	3.000E+00	100	F300	1 0 0 0 1	
3.001E-02	3.488E+00	110	E029	1 2 0 1 1	
3.060E-02	3.556E+00	110	F001	1 0 1 0 2	
3.685E-02	4.282E+00	120	E029	1 2 0 1 1	

(*continued*)

1316. $C_7H_{16}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.537E-02	5.272E+00	130	E029	1 2 0 1 1	
5.557E-02	6.458E+00	140	E029	1 2 0 1 1	
6.830E-02	7.937E+00	150	E029	1 2 0 1 1	
8.352E-02	9.705E+00	160	E029	1 2 0 1 1	
1.046E-01	1.215E+01	170	E029	1 2 0 1 2	
1.355E-01	1.575E+01	180	E029	1 2 0 1 2	
1.753E-01	2.038E+01	190	E029	1 2 0 1 2	
2.213E-01	2.572E+01	200	E029	1 2 0 1 2	
2.894E-01	3.363E+01	210	E029	1 2 0 1 2	
3.847E-01	4.471E+01	220	E029	1 1 0 1 2	
5.404E-01	6.279E+01	230	E029	1 2 0 1 2	
7.894E-01	9.173E+01	240	E029	1 2 0 1 2	
1.054E+00	1.225E+02	245	E029	1 2 0 1 2	
1.029E-02	1.195E+00	ns	H012	0 2 2 0 2	
1.558E-02	1.810E+00	ns	L003	0 0 2 1 2	

1317. $C_7H_{16}O$

Isopropyl *tert*-butyl ether
2-Methyl-2-(1-methylethoxy)-propane
t-Butyl isopropyl ether

RN: 17348-59-3 **MP** (°C)**:** –88
MW: 116.20 **BP** (°C)**:** 87.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.303E-03	5.000E-01	25	K072	1 0 1 1 1	
4.303E-03	5.000E-01	25	M087	1 1 2 1 1	

1318. $C_7H_{16}O$

Heptanol

RN: 53535-33-4 **MP** (°C)**:** –36
MW: 116.20 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.173E+01	20	S006	1 0 0 0 2	
1.240E-02	1.441E+00	24	H345	0 0 0 0 0	

1319. $C_7H_{16}O$

4-Heptanol
Dipropyl carbinol

RN: 589-55-9 **MP** (°C)**:** –42
MW: 116.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.090E-02	4.753E+00	20	H330	0 0 0 0 0	

1320. $C_7H_{16}O$
2,3-Dimethyl-3-pentanol
2,3-Dimethylpentanol-3
RN: 595-41-5 **MP** (°C)**:** <25
MW: 116.20 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	1.836E+01	20	G006	1 2 1 1 2	
1.389E-01	1.614E+01	25	G006	1 2 1 1 2	
1.213E-01	1.410E+01	30	G006	1 2 1 1 2	

1321. $C_7H_{16}O_4S_2$
Sulfonmethane
Sulfonal
RN: 115-24-2 **MP** (°C)**:** 125
MW: 228.33 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.962E-02	1.361E+01	16	A072	1 0 1 0 2	
5.956E-02	1.360E+01	16	F300	1 0 0 0 2	
1.027E-02	2.345E+00	18	F062	1 0 2 2 2	
2.847E-01	6.500E+01	100	F300	1 0 0 0 1	
5.888E-02	1.345E+01	ns	R427	0 0 0 0 0	

1322. $C_7H_{16}O_7$
(+)-Perseitol
D-Manno-α-heptit
RN: 527-06-0 **MP** (°C)**:** 188
MW: 212.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.044E-01	6.460E+01	18	F300	1 0 0 0 2	
1.466E+00	3.110E+02	74	F300	1 0 0 0 1	

1323. $C_7H_{17}O_2PS_3$
Phorate
Thimet
Rampart
Phosphorodithioic acid *O,O*-diethyl *S*-[(ethylthio)methyl] ester
American Cyanamid 3911
CL 35024
RN: 298-02-2 **MP** (°C)**:** –43
MW: 260.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-05	1.790E-02	20	B169	2 1 1 1 1	
1.905E-04	4.961E-02	20	B179	0 0 0 0 0	

(*continued*)

1323. $C_7H_{17}O_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.681E-05	2.000E-02	24	F179	2 2 2 2 2	
2.688E-04	7.000E-02	ns	M061	0 0 0 0 1	
1.920E-04	5.000E-02	rt	M161	0 0 0 0 1	

1324. $C_7H_{17}O_2PS_3$

S-2-Isopropylthioethyl *O,O*-dimethyl phosphorodithioate
Isothioate
O,O-Dimethyls-isopropylthioethyl phosphoroditjioate
RN: 36614-38-7 **MP** (°C)**:**
MW: 260.38 **BP** (°C)**:** 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.725E-04	9.700E-02	25	M161	1 0 0 0 1	
3.725E-04	9.700E-02	25	N304	1 0 0 0 1	

1325. $C_7H_{17}O_4PS_3$

Phorate sulfone
O,O′-Diethyl *S*-ethylsulfonylmethyl-phosphorodithioate
Thimet sulfone
CL 18161
Phosphorodithioic acid *O,O*-diethyl *S*-[(ethylsulfonyl)methyl] ester
RN: 2588-04-7 **MP** (°C)**:**
MW: 292.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E-03	8.593E-01	19	B169	2 0 1 1 2	

1326. $C_8H_2Cl_4N_2$

Chlorquinox
5,6,7,8-Tetrachloroquinoxaline
Lucel
Tetrachloroquinoxaline
RN: 3495-42-9 **MP** (°C)**:** 190
MW: 267.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.732E-06	1.000E-03	25	M161	1 0 0 0 0	

1327. $C_8H_2Cl_4O_4$
Tetrachlorophthalic acid
Tetrachlorphthalsaeure
Tetrachloro-1,2-benzenedicarboxylic acid
RN: 632-58-6 **MP** (°C)**:**
MW: 303.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-02	5.700E+00	14	F300	1 0 0 0 1	
1.007E-01	3.060E+01	99	F300	1 0 0 0 2	

1328. $C_8H_3Cl_2F_3N_2$
Chlorflurazole
4,5-Dichloro-2-(trifluoromethyl)-benzimidazole
Dichloro-2-(trifluoromethyl)benzimidazole
2-Trifluoromethyl-4,5-dichlorobenzimidazole
RN: 3615-21-2 **MP** (°C)**:**
MW: 255.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-04	6.000E-02	ns	B100	0 0 0 0 0	
2.353E-04	6.000E-02	ns	M061	0 0 0 0 1	

1329. $C_8H_3Cl_5O_2$
Pentachlorophenyl acetate
Pentachlorophenol acetate
Rabcon
RN: 1441-02-7 **MP** (°C)**:**
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-05	2.000E-02	ns	L311	0 0 0 0 1	

1330. $C_8H_3Cl_5O_3$
2,3,4,5,6-Pentachlorophenoxyacetic acid
Pentachlorophenoxyacetic acid
RN: 2877-14-7 **MP** (°C)**:**
MW: 324.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	5.839E-02	25	L030	1 0 2 1 1	

1331. $C_8H_4Cl_4O_3$
2,3,4,6-Tetrachlorophenoxyacetic acid
Acetic acid, (2,3,4,6-tetrachlorophenoxy)-
RN: 10587-37-8 **MP** (°C)**:**
MW: 289.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.131E-01	25	L030	1 0 2 1 1	

1332. $C_8H_4N_2$
1,4-Benzenedicarbonitrile
Terephthalonitrile
1,4-Dicyanobenzene
RN: 623-26-7 **MP** (°C)**:**
MW: 128.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.970E-04	8.931E-02	25	C316	0 0 0 0 0	0.1M NaCl

1333. $C_8H_4N_2S$
m-Cyanophenyl isothiocyanate
3-Isothiocyanato-benzonitrile
3-Cyanophenyl isothiocyanate
RN: 3125-78-8 **MP** (°C)**:**
MW: 160.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.410E-04	1.027E-01	25	K032	2 2 0 1 2	

1334. $C_8H_4N_2S_2$
m-Isothiocyanophenyl isothiocyanate
3-Isothiocyanophenyl isothiocyanate
RN: 3125-77-7 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.845E-03	25	K032	2 2 0 1 1	

1335. $C_8H_4O_3$
Phthalic anhydride
1,2-Benzenedicarboxylic acid anhydride
1,3-Isobenzofurandione
Phthalic acid anhydride
1,3-Dioxophthalan
1,3 Phthalandione
RN: 85-44-9 **MP** (°C)**:** 130.8
MW: 148.12 **BP** (°C)**:** 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-02	6.200E+00	26.70	L095	2 2 1 1 2	
4.027E-02	5.964E+00	rt	D021	0 0 1 1 2	

1336. $C_8H_5ClO_4$
3-Chlorophthalic acid
3-Chlor-phthalsaeure
RN: 27563-65-1 **MP** (°C)**:**
MW: 200.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-01	2.120E+01	14	F300	1 0 0 0 2	

1337. $C_8H_5Cl_3O_2$
Chlorfenac
2,3,6-Trichlorophenylacetic acid
Fenac
RN: 85-34-7 **MP** (°C)**:** 161
MW: 239.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.351E-04	2.000E-01	28	M161	1 0 0 0 2	
8.351E-04	2.000E-01	30	M061	1 0 0 0 2	

1338. $C_8H_5Cl_3O_3$
2,4,5-Trichlorophenoxyacetic acid
Acetic acid, (2,4,5-trichlorophenoxy)-
(2,4,5-Trichlorophenoxy)acetic acid
2,4,5-T
RN: 93-76-5 **MP** (°C)**:** 156
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.316E-04	2.380E-01	20	B185	0 0 0 0 0	
7.398E-04	1.890E-01	20	M061	1 0 0 0 2	
1.090E-03	2.785E-01	24.99	N417	0 0 0 0 0	

(*continued*)

1338. $C_8H_5Cl_3O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.810E-01	25	B164	1 0 1 1 2	
1.096E-03	2.800E-01	25	B185	0 0 0 0 0	
1.050E-03	2.683E-01	25	L030	1 0 2 1 2	
1.088E-03	2.780E-01	25	M161	1 0 0 0 2	
9.316E-04	2.380E-01	30	B200	1 0 0 0 2	
9.783E-04	2.499E-01	ns	B100	0 0 0 0 1	
7.828E-04	2.000E-01	ns	B185	0 0 0 0 0	
8.000E-04	2.044E-01	ns	F184	0 0 0 0 1	
9.316E-04	2.380E-01	ns	K138	0 0 0 0 1	
9.824E-04	2.510E-01	ns	L024	0 0 0 0 2	
2.512E-04	6.418E-02	ns	M163	0 0 0 0 0	EFG
7.828E-04	2.000E-01	ns	N013	0 0 0 0 2	

1339. $C_8H_5Cl_3O_3$
3,4,5-Trichlorophenoxyacetic acid
Acetic acid, (3,4,5-trichlorophenoxy)-
3,4,5-T
RN: 80496-87-3 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	2.938E-01	25	L030	1 0 2 1 2	

1340. $C_8H_5Cl_3O_3$
2,3,4-Trichlorophenoxyacetic acid
Acetic acid, (2,3,4-trichlorophenoxy)-
2,3,4-T
RN: 25141-27-9 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	2.044E-01	25	L030	1 0 2 1 1	

1341. $C_8H_5Cl_3O_3$
2,4,6-Trichlorophenoxyacetic acid
Acetic acid, (2,4,6-trichlorophenoxy)-
2,4,6-T
RN: 575-89-3 **MP** (°C)**:** 45
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	2.478E-01	25	L030	1 0 2 1 1	

1342. $C_8H_5Cl_3O_3$
2,3,6-Trichlorophenoxyacetic acid
Acetic acid, (2,3,6-trichlorophenoxy)-
2,3,6-T
RN: 4007-00-5 **MP** (°C)**:** 148
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	6.132E-01	25	L030	1 0 2 1 2	

1343. $C_8H_5Cl_3O_3$
2,3,5-Trichlorophenoxyacetic acid
Acetic acid, (2,3,5-trichlorophenoxy)-
2,3,5-T
RN: 33433-95-3 **MP** (°C)**:**
MW: 255.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.555E-01	25	L030	1 0 2 1 2	

1344. $C_8H_5F_3O$
2,2,2-Trifluoroacetophenone
Trifluoroacetophenone
α,α,α-Trifluoroacetophenone
Phenyl trifluoromethyl ketone
2,2,2-Trifluoro-1-phenylethanone
RN: 434-45-7 **MP** (°C)**:** –40
MW: 174.12 **BP** (°C)**:** 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.007E-02	1.220E+01	30	B433	0 0 0 0 0	

1345. $C_8H_5F_3O_2$
α,α,α-Trifluoro-*o*-toluic acid
Trifluoro-*o*-toluic acid
Acide orthotrifluortoluique
RN: 433-97-6 **MP** (°C)**:** 111
MW: 190.12 **BP** (°C)**:** 247

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	4.800E+00	25	D064	1 2 1 1 2	

1346. $C_8H_5NO_2$
Phthalimide
Phthalimid
RN: 85-41-6 **MP** (°C)**:** 238.0
MW: 147.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.447E-03	3.600E-01	25	F300	1 0 0 0 1	
2.719E-02	4.000E+00	100	F300	1 0 0 0 0	
4.075E-03	5.996E-01	rt	D021	0 0 1 1 0	

1347. $C_8H_5NO_2S$
3-Carboxyphenylisothiocyanate
m-Isothiocyanobenzoic acid
RN: 2131-63-7 **MP** (°C)**:**
MW: 179.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-04	1.004E-01	25	D019	1 1 1 1 2	
8.000E-04	1.434E-01	25	K032	2 2 0 1 1	

1348. $C_8H_5NO_2S$
4-Carboxyphenylisothiocyanate
p-Carboxyphenylisothiocyanate
RN: 2131-62-6 **MP** (°C)**:**
MW: 179.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	1.900E-02	25	D019	1 1 1 1 2	

1349. $C_8H_5NO_4$
6-Nitrophthalide
6-Nitro-phthalid
RN: 610-93-5 **MP** (°C)**:** 145
MW: 179.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-03	4.000E-01	25	F300	1 0 0 0 2	

1350. $C_8H_5NO_6$
3-Nitrophthalic acid
3-Nitro-phthalsaeure
RN: 603-11-2 **MP** (°C)**:** 218
MW: 211.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.520E-02	2.010E+01	25	F300	1 0 0 0 2	

1351. $C_8H_5NO_6$
2,3,4-Pyridinetricarboxylic acid
Pyridin-tricarbonsaeure-(2,3,4)
RN: 632-95-1 **MP** (°C)**:** 250
MW: 211.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.684E-02	1.200E+01	15	F300	1 0 0 0 1	

1352. C_8H_6
Ethynylbenzene
Phenylacetylene
RN: 536-74-3 **MP** (°C)**:** –44.8
MW: 102.14 **BP** (°C)**:** 142.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.467E-03	4.562E-01	ns	D001	0 0 0 0 2	

1353. C_8H_6BrNS
3-Bromobenzyl isothiocyanate
m-Bromobenzyl isothiocyanate
RN: 3845-33-8 **MP** (°C)**:**
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.441E-02	25	D014	1 0 0 0 1	

1354. C_8H_6BrNS
4-Bromobenzyl isothiocyanate
p-Bromobenzyl isothiocyanate
RN: 2076-56-4 **MP** (°C)**:**
MW: 228.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.483E-02	25	D014	1 0 0 0 1	
1.500E-04	3.422E-02	25	D019	1 1 1 1 2	

1355. C_8H_6ClNS
3-Chlorobenzyl isothiocyanate
m-Chlorobenzyl isothiocyanate
RN: 3694-58-4 **MP** (°C)**:**
MW: 183.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	2.516E-02	25	D014	1 0 0 0 1	

1356. C_8H_6ClNS
4-Chlorobenzyl isothiocyanate
p-Chlorobenzyl isothiocyanate
RN: 3694-45-9 **MP** (°C)**:**
MW: 183.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	2.718E-02	25	D014	1 0 0 0 1	

1357. $C_8H_6Cl_2O_3$
2,4-Dichlorophenoxyacetic acid
2,4-D
(2,4-Dichlorophenoxy)acetic acid
RN: 94-75-7 **MP** (°C)**:** 138
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.805E-03	6.200E-01	20	F311	1 2 2 2 1	
2.443E-03	5.400E-01	20	M061	1 0 0 0 2	
2.939E-03	6.496E-01	21.50	B200	1 0 0 0 0	
4.072E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.060E-03	6.764E-01	24.99	N417	0 0 0 0 0	
3.085E-03	6.820E-01	25	B164	1 0 1 1 2	
3.280E-03	7.250E-01	25	B185	0 0 0 0 0	
4.026E-03	8.900E-01	25	F071	1 1 2 1 2	
2.360E-03	5.217E-01	25	L030	1 0 2 1 2	
2.805E-03	6.200E-01	25	M161	1 0 0 0 2	
2.713E-03	5.996E-01	ns	B100	0 0 0 0 0	
4.072E-03	9.000E-01	ns	B185	0 0 0 0 0	
1.810E-03	4.000E-01	ns	B185	0 0 0 0 0	
2.500E-03	5.526E-01	ns	F184	0 0 0 0 1	
4.072E-03	9.000E-01	ns	K138	0 0 0 0 1	
2.805E-03	6.200E-01	ns	L024	0 0 0 0 2	
4.298E-03	9.500E-01	ns	M110	0 0 0 0 0	EFG
1.259E-03	2.783E-01	ns	M163	0 0 0 0 0	EFG
4.026E-03	8.900E-01	ns	M344	0 0 0 0 2	
2.488E-03	5.500E-01	ns	N013	0 0 0 0 2	

1358. $C_8H_6Cl_2O_3$
Dicamba
2-Methoxy-3,6-dichlorobenzoic acid
RN: 1918-00-9 **MP** (°C)**:** 98
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.036E-02	4.500E+00	25	B200	1 0 0 0 1	
2.036E-02	4.500E+00	25	M161	1 0 0 0 1	
3.591E-02	7.937E+00	ns	B100	0 0 0 0 0	

1359. $C_8H_6Cl_2O_3$
3,5-Dichlorophenoxyacetic acid
3,5-D
RN: 587-64-4 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-03	9.615E-01	25	L030	1 0 2 1 2	

1360. $C_8H_6Cl_2O_3$
3,4-Dichlorophenoxyacetic acid
3,4-D
RN: 588-22-7 **MP** (°C)**:** 138
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-03	4.576E-01	25	L030	1 0 2 1 2	
2.090E-03	4.620E-01	ns	B185	0 0 0 0 0	

1361. $C_8H_6Cl_2O_3$
2,6-Dichlorophenoxyacetic acid
2,6-D
RN: 575-90-6 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-03	1.558E+00	25	L030	1 0 2 1 2	

1362. $C_8H_6Cl_2O_3$
2,3-Dichlorophenoxyacetic acid
2,3-D
RN: 2976-74-1 **MP** (°C)**:** 173
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-03	3.426E-01	25	L030	1 0 2 1 2	

1363. $C_8H_6Cl_2O_3$
2,5-Dichlorophenoxyacetic acid
2,5-D
RN: 582-54-7 **MP** (°C)**:**
MW: 221.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-03	5.349E-01	25	L030	1 0 2 1 2	

1364. $C_8H_6Cl_4O_2$
Tetrachloroveratrole
3,4,5,6-Tetrachloro-1,2-dimethoxybenzene
RN: 944-61-6 **MP** (°C)**:**
MW: 275.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.762E-06	1.590E-03	25	L348	1 2 2 1 2	

1365. $C_8H_6Cl_5NO_2$
Penclomedine
Pyridine
3,5-Dichloro-2,4-dimethoxy-6-(trichloromethyl)
NSC 338720
RN: 108030-77-9 **MP** (°C)**:**
MW: 325.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.229E-06	4.000E-04	25	P325	0 0 0 0 0	
1.229E-06	4.000E-04	25	P336	0 0 0 0 0	

1366. $C_8H_6F_3N_3O_4S_2$
Flumethiazide
6-(Trifluoromethyl)-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
6-Trifluoromethyl-7-sulfamoyl-4H-1,2,4-benzothiadiazine 1,1-dioxide
Trifluoromethylthiazide
RN: 148-56-1 **MP** (°C)**:**
MW: 329.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.189E-03	1.050E+00	rt	A095	0 0 2 2 2	

1367. C_8H_6INS
3-Iodobenzyl isothiocyanate
m-Iodobenzyl isothiocyanate
RN: 3696-68-2 **MP** (°C)**:**
MW: 275.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	1.513E-02	25	D014	1 0 0 0 1	

1368. C_8H_6INS
4-Iodobenzyl isothiocyanate
p-Iodobenzyl isothiocyanate
RN: 3694-49-3 **MP** (°C)**:**
MW: 275.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-05	1.403E-02	25	D014	1 0 0 0 1	

1369. $C_8H_6N_2O_2S$
3-Nitrobenzyl isothiocyanate
m-Nitrobenzyl isothiocyanate
RN: 3696-69-3 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.593E-02	25	D014	1 0 0 0 1	

1370. $C_8H_6N_2O_2S$
4-Nitrobenzyl isothiocyanate
p-Nitrobenzyl isothiocyanate
RN: 3694-47-1 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	4.525E-02	25	D014	1 0 0 0 1	

1371. $C_8H_6N_4O_5$
Nitrofurantoin
1-[(5-Nitrofurfurylidene)amino]hydantoin
Furatoin
Macrodantin
Macrobid
Welfurin
RN: 67-20-9 **MP** (°C)**:** 268
MW: 238.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.619E-04	1.100E-01	22	B154	1 1 1 1 1	pH 3.5
3.338E-04	7.950E-02	24	C034	2 0 2 2 2	
3.338E-04	7.950E-02	24	C118	1 0 0 0 2	
5.207E-04	1.240E-01	25	M457	0 0 0 0 0	
4.753E-04	1.132E-01	30	C011	2 0 2 1 0	EFG
4.761E-04	1.134E-01	30	C034	2 0 2 2 2	
4.761E-04	1.134E-01	30	C118	1 0 0 0 2	
8.264E-04	1.968E-01	37	A330	0 0 0 0 0	
1.142E-03	2.720E-01	37	B044	2 2 2 1 2	pH 7.2
7.310E-04	1.741E-01	37	C011	2 0 2 1 0	EFG
7.310E-04	1.741E-01	37	C034	2 0 2 2 2	
7.310E-04	1.741E-01	37	C118	1 0 0 0 2	
5.878E-04	1.400E-01	37	E044	1 0 1 1 2	
6.508E-04	1.550E-01	37	P034	1 0 0 0 2	pH 5
1.055E-03	2.512E-01	45	C034	2 0 2 2 2	
1.055E-03	2.512E-01	45	C118	1 0 0 0 2	
7.978E-04	1.900E-01	ns	K444	0 0 0 0 0	
5.249E-04	1.250E-01	ns	P033	0 0 0 0 2	
5.248E-04	1.250E-01	ns	R427	0 0 0 0 0	

1372. $C_8H_6N_4O_8$
Alloxantin
Uroxine
Alloxantin hydrate
RN: 76-24-4 **MP** (°C)**:** 254dec
MW: 286.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-03	5.017E-01	25	B119	1 0 2 2 0	EFG
1.013E-02	2.900E+00	25	F300	1 0 0 0 1	
2.097E-01	6.000E+01	100	F300	1 0 0 0 0	

1373. $C_8H_6N_4S_2$
Methylthiobenzothiazole
Benzothiazole
RN: 76006-86-5 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-04	1.100E-01	22	P323	0 0 0 0 0	

1374. $C_8H_6O_2$
Phthalic dicarboxaldehyde
o-Phthalaldehyd
RN: 643-79-8 **MP** (°C)**:** 56.5
MW: 134.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-01	1.400E+01	h	F300	0 0 0 0 1	

1375. $C_8H_6O_2$
Terephthaldicarboxaldehyde
Terephthalaldehyd
RN: 623-27-8 **MP** (°C)**:** 115
MW: 134.14 **BP** (°C)**:** 246.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	2.000E-01	20	F300	1 0 0 0 0	
1.297E-01	1.740E+01	100	F300	1 0 0 0 1	

1376. $C_8H_6O_3$
Piperonal
Heliotropine
3,4-Dihydroxybenzaldehyde methylene ketal
Methylenedioxy procatechuic aldehyde
Protocatechuic aldehyde methylene ether
Piperonyl aldehyde
RN: 120-57-0 **MP** (°C)**:** 37
MW: 150.14 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-02	3.500E+00	20	F300	1 0 0 0 1	
4.463E-02	6.700E+00	78	F300	1 0 0 0 1	

1377. $C_8H_6O_3$

Benzoylformic acid
Phenyglyoxilic acid
RN: 611-73-4 **MP** (°C)**:** 67
MW: 150.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.128E+00	9.200E+02	0	C020	1 2 1 1 1	

1378. $C_8H_6O_4$

1,4-Benzenedicarboxylic acid
Terephthalic acid
p-Phthalic acid
RN: 100-21-0 **MP** (°C)**:**
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.029E-05	1.500E-02	20	F300	1 0 0 0 1	
1.920E-03	3.190E-01	25	C316	0 0 0 0 0	0.1M HCL
6.019E-04	9.999E-02	80	A027	1 0 0 0 0	

1379. $C_8H_6O_4$

1,2-Benzenedicarboxylic acid
o-Phthalic acid
Phthalic acid
Phthalsaeure
Benzene-1,2-dicarboxylic acid
RN: 88-99-3 **MP** (°C)**:** 230
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.295E+00	0	M043	1 0 0 0 1	
2.219E-02	3.686E+00	2	A027	1 0 0 0 1	
2.159E-02	3.587E+00	10	M043	1 0 0 0 1	
7.935E-03	1.318E+00	10	S198	2 1 2 2 2	
1.571E-02	2.611E+00	10.49	A341	0 0 0 0 0	
3.471E-02	5.767E+00	20	A027	1 0 0 0 1	
3.435E-02	5.707E+00	20	F069	2 2 2 2 2	
3.431E-02	5.700E+00	20	F300	1 0 0 0 1	
3.352E-02	5.569E+00	20	M043	1 0 0 0 1	
7.214E-03	1.199E+00	20	S198	2 1 2 2 2	
3.915E-02	6.504E+00	22.99	A341	0 0 0 0 0	
4.200E-02	6.978E+00	24.99	A341	0 0 0 0 0	
8.600E-02	1.429E+01	25	H084	1 0 0 0 1	
8.520E-02	1.415E+01	25	K040	1 0 2 1 2	
4.192E-02	6.965E+00	25	M030	2 1 0 1 2	
4.279E-02	7.109E+00	25.8	W029	1 2 1 1 2	
4.808E-02	7.988E+00	28	D050	1 2 1 2 2	
5.152E-02	8.560E+00	29.49	A341	0 0 0 0 0	

(*continued*)

1379. $C_8H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	8.141E+00	30	H019	0 0 0 0 0	
4.777E-02	7.937E+00	30	M043	1 0 0 0 0	
8.235E-03	1.368E+00	30	S198	2 1 2 2 2	
5.865E-02	9.743E+00	33.99	A341	0 0 0 0 0	
6.033E-02	1.002E+01	35	M030	2 1 0 1 2	
6.561E-02	1.090E+01	35.99	A341	0 0 0 0 0	
6.925E-02	1.150E+01	37.99	A341	0 0 0 0 0	
7.137E-02	1.186E+01	40	M043	1 0 0 0 1	
8.274E-02	1.375E+01	41.99	A341	0 0 0 0 0	
7.865E-02	1.307E+01	43.7	W029	1 2 1 1 2	
8.981E-02	1.492E+01	43.99	A341	0 0 0 0 0	
8.991E-02	1.494E+01	44.99	A341	0 0 0 0 0	
8.580E-02	1.425E+01	45	M030	2 1 0 1 2	
9.890E-02	1.643E+01	45.99	A341	0 0 0 0 0	
9.753E-02	1.620E+01	48.9	W029	1 2 1 1 2	
1.212E-01	2.014E+01	49.99	A341	0 0 0 0 0	
1.116E-01	1.854E+01	49.99	A341	0 0 0 0 0	
1.349E-01	2.241E+01	53.99	A341	0 0 0 0 0	
1.277E-01	2.122E+01	55	M030	2 1 0 1 2	
1.339E-01	2.225E+01	58.0	W029	1 2 1 1 2	
1.639E-01	2.724E+01	60	M043	1 0 0 0 1	
1.741E-01	2.892E+01	60.99	A341	0 0 0 0 0	
1.695E-01	2.815E+01	63.7	W029	1 2 1 1 2	
2.145E-01	3.564E+01	64.99	A341	0 0 0 0 0	
1.892E-01	3.144E+01	65	M030	2 1 0 1 2	
2.826E-01	4.695E+01	75	M030	2 1 0 1 2	
3.042E-01	5.053E+01	77.8	W029	1 2 1 1 2	
3.567E-01	5.927E+01	80	M043	1 0 0 0 1	
4.334E-01	7.200E+01	85	F300	1 0 0 0 0	
4.297E-01	7.138E+01	85	M030	2 1 0 1 2	
4.248E-01	7.058E+01	85.7	W029	1 2 1 1 2	
6.377E-01	1.059E+02	94.8	W029	1 2 1 1 2	
9.182E-01	1.525E+02	100	M043	1 0 0 0 2	
8.208E-01	1.364E+02	101.1	W029	1 2 1 1 2	
1.370E+00	2.276E+02	113.8	W029	1 2 1 1 2	
9.015E-03	1.498E+00	ns	F014	0 0 0 0 2	
2.458E-02	4.083E+00	rt	H431	0 0 0 0 0	

1380. $C_8H_6O_4$

Isophthalic acid
1,3-Benzenedicarboxylic acid
m-Phthalic acid

RN: 121-91-5 **MP** (°C)**:** 345
MW: 166.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.611E-04	6.000E-02	2	A027	1 0 0 0 0	
6.019E-04	9.999E-02	20	A027	1 0 0 0 0	

(*continued*)

1380. $C_8H_6O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-03	1.811E-01	28.29	L437	0 0 0 0 0	
1.656E-03	2.752E-01	40.99	L437	0 0 0 0 0	
2.535E-03	4.212E-01	51.99	L437	0 0 0 0 0	
4.021E-03	6.681E-01	64.99	L437	0 0 0 0 0	
6.260E-03	1.040E+00	76.49	L437	0 0 0 0 0	
6.013E-03	9.990E-01	80	A027	1 0 0 0 0	
8.300E-03	1.379E+00	83.49	L437	0 0 0 0 0	
9.441E-03	1.568E+00	86.47	L437	0 0 0 0 0	
1.286E-02	2.137E+00	93.42	L437	0 0 0 0 0	
4.610E-04	7.659E-02	rt	H431	0 0 0 0 0	

1381. $C_8H_6O_5$

2-Hydroxyisophthalic acid
2-Hydroxy-*iso*-phthalsaeure

RN: 606-19-9 **MP** (°C)**:** 244
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-01	2.640E+01	100	F300	1 0 0 0 2	

1382. $C_8H_6O_5$

4-Hydroxyisophthalic acid
4-Hydroxy-*iso*-phthasaeure

RN: 636-46-4 **MP** (°C)**:** 310
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.647E-03	3.000E-01	24	F300	1 0 0 0 1	

1383. $C_8H_6O_5$

5-Hydroxyisophthalic acid
5-Hydroxy-*iso*-phthalsaeure

RN: 618-83-7 **MP** (°C)**:** 293
MW: 182.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.294E-03	6.000E-01	15	F300	1 0 0 0 1	
8.889E-01	1.619E+02	99	F300	1 0 0 0 2	

1384. C_8H_6S

Thianaphthene
Benzo[b]thiophene
Benzothiofuran
1-Benzothiophene

RN: 95-15-8 **MP** (°C)**:** 29–32
MW: 134.20 **BP** (°C)**:** 221–222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-03	2.162E-01	59.0	L339	2 0 2 2 2	
2.610E-03	3.503E-01	78.5	L339	2 0 2 2 2	
4.386E-03	5.886E-01	99.0	L339	2 0 2 2 2	

1385. $C_8H_7BrN_2O_3$

o-Nitro-*o*-bromacetanilide
2-Bromo-5-nitroacetanilide

RN: 245115-83-7 **MP** (°C)**:**
MW: 259.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.720E-02	2.000E+01	rt	F043	0 0 2 1 1	

1386. $C_8H_7BrN_2O_3$

p-Nitro-*o*-bromacetanilide
2-Bromo-4-nitroacetanilide

RN: 57045-86-0 **MP** (°C)**:**
MW: 259.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.832E-02	1.770E+01	rt	F043	0 0 2 1 2	

1387. $C_8H_7ClN_2O_3$

p-Nitro-*o*-chloracetanilide
2-Chloro-4-nitroacetanilide

RN: 881-87-8 **MP** (°C)**:**
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1388. $C_8H_7ClN_2O_3$
o-Nitro-*o*-chloracetanilide
2-Chloro-5-nitroacetanilide
RN: 72487-80-0 **MP** (°C)**:**
MW: 214.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1389. $C_8H_7ClO_3$
4-Chlorophenoxyacetic acid
4-CPA
p-Chlorophenoxyacetic acid
RN: 122-88-3 **MP** (°C)**:** 157
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.545E-03	8.480E-01	25	B164	1 0 1 1 2	
2.042E-03	3.810E-01	25	B185	0 0 0 0 0	
5.130E-03	9.572E-01	25	L030	1 0 2 1 2	

1390. $C_8H_7ClO_3$
3-Chlorophenoxyacetic acid
m-Chlorophenoxyacetic acid
RN: 588-32-9 **MP** (°C)**:**
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E-02	2.360E+00	25	L030	1 0 2 1 2	

1391. $C_8H_7ClO_3$
2-Chlorophenoxyacetic acid
o-Chlorophenoxyacetic acid
RN: 614-61-9 **MP** (°C)**:** 146
MW: 186.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.850E-03	1.278E+00	25	L030	1 0 2 1 2	

1392. $C_8H_7Cl_2NO_2$
Chloramben methyl ester
Vegiben 2E
Methyl 3-amino-2,5-dichlorobenzoate
Amchem 65-81-B
Methyl chloramben
Chloramben methyl
RN: 7286-84-2 **MP** (°C)**:** 63.5
MW: 220.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.453E-04	1.200E-01	20	M161	1 0 0 0 2	

1393. $C_8H_7Cl_3O$
2,4,6-Trichloro-3,5-dimethyl-phenol
3,5-Xylenol, 2,4,6-trichloro-
RN: 6972-47-0 **MP** (°C)**:**
MW: 225.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	4.961E-03	25	B316	0 0 0 0 0	

1394. $C_8H_7Cl_3O_2$
3,4,5-Trichloroveratrole
4,5,6-Trichloroveratrole
RN: 16766-29-3 **MP** (°C)**:** 66
MW: 241.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.265E-05	1.030E-02	25	L348	1 2 2 1 2	

1395. C_8H_7N
Indole
2,3-Benzopyrrole
Benzopyrrole
1-Benzazole
1-Benzol β pyrrol
RN: 120-72-9 **MP** (°C)**:** 52
MW: 117.15 **BP** (°C)**:** 253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.219E-02	1.080E+01	25	K119	1 0 0 0 2	
3.037E-02	3.558E+00	25	P051	2 1 1 2 2	
3.037E-02	3.558E+00	25.00	P007	2 1 2 2 2	

1396. C_8H_7N
p-Toluonitrile
p-Cyanotoluene
p-Methylbenzonitrile
4-Methylbenzenecarbonitrile
RN: 104-85-8 **MP** (°C)**:**
MW: 117.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.523E+00	25	M327	1 0 0 1 2	

1397. C_8H_7NOS
m-Methoxyphenyl isothiocyanate
3-Methoxyphenyl isothiocyanate
RN: 3125-64-2 **MP** (°C)**:**
MW: 165.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	4.461E-02	25	K032	2 2 0 1 2	

1398. C_8H_7NOS
p-Methoxyphenyl isothiocyanate
4-Methoxyphenylisothiocyanate
RN: 2284-20-0 **MP** (°C)**:** 18.0
MW: 165.22 **BP** (°C)**:** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	4.130E-02	25	D019	1 1 1 1 2	

1399. $C_8H_7NO_3$
Oxanilic acid
N-Phenyloxalic acid monoamide
Oxanilsaure
RN: 500-72-1 **MP** (°C)**:** 150
MW: 165.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.990E-02	8.241E+00	25	D058	1 0 1 1 2	

1400. $C_8H_7NO_4$
6-Nitro-3-methylbenzoic acid
2-Nitro-5-methylbenzoic acid
5-Methyl-2-nitrobenzoic acid
3-Methyl-6-nitrobenzoic acid
RN: 3113-72-2 **MP** (°C)**:**
MW: 181.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.043E-02	3.700E+00	10	G063	1 0 0 0 1	
2.595E-02	4.700E+00	20	G063	1 0 0 0 1	
9.385E-02	1.700E+01	40	G063	1 0 0 0 1	
9.937E-02	1.800E+01	50	G063	1 0 0 0 1	
1.490E-01	2.700E+01	60	G063	1 0 0 0 1	
1.932E-01	3.500E+01	65	G063	1 0 0 0 1	
2.484E-01	4.500E+01	70	G063	1 0 0 0 1	
3.643E-01	6.600E+01	80	G063	1 0 0 0 1	
3.699E-01	6.700E+01	100	G063	1 0 0 0 1	

1401. $C_8H_7NO_4$
2-Nitro-3-methylbenzoic acid
2-Nitro-*m*-toluic acid
3-Methyl-2-nitrobenzoic acid
RN: 5437-38-7 **MP** (°C)**:**
MW: 181.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.208E-03	4.000E-01	20	G063	1 0 0 0 1	
8.832E-03	1.600E+00	40	G063	1 0 0 0 1	
3.202E-02	5.800E+00	80	G063	1 0 0 0 1	
3.312E-02	6.000E+00	100	G063	1 0 0 0 0	

1402. C_8H_7NS
Benzyl isothiocyanate
Benzylisothiocyanate
Isothiocyanatomethylbenzene
RN: 622-78-6 **MP** (°C)**:** 112
MW: 149.22 **BP** (°C)**:** 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.089E-01	25	D014	1 0 0 0 2	

1403. C_8H_7NS
p-Tolyl isothiocyanate
4-Tolylisothiocyanate
RN: 622-59-3 **MP** (°C)**:** 25
MW: 149.22 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	2.835E-03	25	D019	1 1 1 1 1	

1404. C_8H_7NS
m-Methylphenyl isothiocyanate
3-Methylphenyl isothiocyanate
RN: 614-69-7 **MP** (°C)**:**
MW: 149.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	2.119E-02	25	K032	2 2 0 1 2	

1405. $C_8H_7N_5O$
7-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.035E-02	7.634E+00	100	A083	1 2 0 0 0	

1406. $C_8H_7N_5O$
2-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	3.226E+01	100	A083	1 2 0 0 0	

1407. $C_8H_7N_5O$
4-Acetamidopteridine
RN: **MP** (°C)**:**
MW: 189.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E+00	3.333E+02	100	A083	1 2 0 0 0	

1408. $C_8H_7N_5O_8$
2,4,6-Trinitrophenylethylnitramine
Tetrethyl
Trinitrophenylethylnitramine
Ethyl tetryl
RN: 6052-13-7 **MP** (°C)**:**
MW: 301.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-04	6.000E-02	22	D067	1 2 0 0 0	
8.633E-04	2.600E-01	50	D067	1 2 0 0 1	
8.998E-03	2.710E+00	100	D067	1 2 0 0 2	

1409. C_8H_8
Styrene
Phenylethylene
Styrolene
Styrol
Ethenylbenzene
Annamene
RN: 100-42-5 **MP** (°C)**:** –30
MW: 104.15 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-03	2.899E-01	7	L028	1 0 1 1 1	
2.400E-03	2.499E-01	15	L028	1 0 1 1 1	
1.152E-03	1.200E-01	20	L096	1 2 0 2 2	
3.167E-03	3.299E-01	24	L028	1 0 1 1 1	
2.880E-03	3.000E-01	25	A002	1 2 1 1 1	
1.540E-03	1.604E-01	25	B173	2 0 2 2 2	
2.975E-03	3.099E-01	25	L028	1 0 1 1 1	
3.455E-03	3.599E-01	32	L028	1 0 1 1 1	
3.839E-03	3.998E-01	40	L028	1 0 1 1 1	
3.839E-03	3.998E-01	44	L028	1 0 1 1 1	
4.319E-03	4.498E-01	49	L028	1 0 1 1 1	
4.319E-03	4.498E-01	51	L028	1 0 1 1 1	
4.798E-03	4.998E-01	56	L028	1 0 1 1 1	
8.658E-02	9.018E+00	65	A324	2 2 2 1 1	
5.566E-03	5.797E-01	65	L028	1 0 1 1 1	

1410. $C_8H_8BrCl_2O_3PS$

Bromophos
O-(4-Bromo-2,5-dichlorophenyl) *O,O*-dimethyl phosphorothioate
Nexion
Brofene
Brophene
Omexan

RN: 2104-96-3 **MP** (°C)**:** 51
MW: 366.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.557E-07	2.400E-04	10	B324	0 0 0 0 0	
6.558E-07	2.400E-04	10	B324	0 0 0 0 0	
8.197E-07	3.000E-04	20	B169	2 1 1 1 1	*sic*
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
2.732E-06	1.000E-03	20	F311	1 2 2 2 1	*sic*
1.093E-04	4.000E-02	20	M061	1 0 0 0 1	
1.093E-04	4.000E-02	20	W311	1 0 0 0 1	
2.634E-06	9.641E-04	30	B324	0 0 0 0 0	
2.623E-06	9.600E-04	30	B324	0 0 0 0 0	
1.093E-04	4.000E-02	ns	E050	0 0 0 0 1	
1.093E-04	4.000E-02	rt	M161	0 0 0 0 1	

1411. C_8H_8BrNO

4′-Bromoacetanilide
Acetamide, *N*-(4-bromophenyl)-
Acetanilide, 4′-bromo-
Bromoantifebrin

RN: 103-88-8 **MP** (°C)**:**
MW: 214.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.498E-01	25	D044	0 0 0 0 0	

1412. C_8H_8ClNO

p-Chloroacetanilide
Acetamide, *N*-(4-chlorophenyl)-
Acetanilide, 4′-chloro-

RN: 539-03-7 **MP** (°C)**:**
MW: 169.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.696E-01	25	D044	0 0 0 0 0	

1413. $C_8H_8Cl_2IO_3PS$

Iodofenphos
O-(2,5-Dichloro-4-iodophenyl) *O,O*-dimethyl phosphorothioate
Nuvanol-N
Dimethyl *O*-2,5-dichloro-4-iodophenyl thiophosphate
Alfacron
Jodfenphos

RN: 18181-70-9 **MP** (°C)**:** 72
MW: 413.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.421E-07	1.000E-04	20	B169	2 1 1 1 1	
4.843E-06	2.000E-03	20	M161	1 0 0 0 0	

1414. $C_8H_8Cl_2O$

2,4-Dichloro-6-ethyl-phenol
Phenol, 2,4-dichloro-6-ethyl-

RN: 24539-94-4 **MP** (°C)**:**
MW: 191.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.484E-01	25	B316	0 0 0 0 0	

1415. $C_8H_8Cl_2O_2$

Chloroneb
Demosan
Terraneb
Terraneb SP
1,4-Dichloro-2,5-dimethoxybenzene
Terraneb B

RN: 2675-77-6 **MP** (°C)**:** 134.5
MW: 207.06 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.864E-05	8.000E-03	25	M161	1 0 0 0 0	

1416. $C_8H_8Cl_2O_2$

4,5-Dichloroveratrole
Benzene, 1,2-dichloro-4,5-dimethoxy-

RN: 2772-46-5 **MP** (°C)**:** 83
MW: 207.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-04	7.230E-02	25	L348	1 2 2 1 2	average of 2

1417. $C_8H_8Cl_3O_3PS$

Ronnel
Fenchlorphos
Dermafos
Dimethyl trichlorophenylthiophosphate

RN: 299-84-3 **MP** (°C)**:** 35
MW: 321.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.866E-06	6.000E-04	20	B169	2 2 1 1 1	
3.359E-06	1.080E-03	20	C053	0 0 0 0 0	
3.110E-06	1.000E-03	20	E048	1 2 1 1 0	
7.775E-06	2.500E-03	20	F311	1 2 2 2 1	
5.287E-06	1.700E-03	ns	F040	1 2 2 2 1	
3.359E-06	1.080E-03	ns	F071	0 1 2 1 2	
1.866E-05	6.000E-03	ns	K138	0 0 0 0 1	
1.368E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.244E-04	4.000E-02	rt	M161	0 0 0 0 1	

1418. C_8H_8FNO

4′-Fluoroacetanilide
Acetamide, *N*-(4-fluorophenyl)-
4-Fluoroacetanilide

RN: 351-83-7 **MP** (°C)**:**
MW: 153.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-02	2.496E+00	25	D044	0 0 0 0 0	

1419. $C_8H_8F_3N_3O_4S_2$

Hydroflumethiazide
Diucardin
Saluron

RN: 135-09-1 **MP** (°C)**:** 272
MW: 331.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-03	4.800E-01	37	C087	0 0 0 0 0	
2.048E-03	6.785E-01	37	C315	0 0 0 0 0	0.1N HCL, average of 4
5.643E-04	1.870E-01	ns	B404	0 2 1 1 0	
9.958E-04	3.299E-01	rt	K144	0 0 0 0 1	

1420. C_8H_8INO
p-Iodoaniline-*N*-acetate
4-Iodanilin-*N*-acetat
4-Iodoacetanilide
Acetanilide, 4′-iodo-
4-Acetamidophenyl iodide
p-Iodoacetanilide
RN: 622-50-4 **MP** (°C)**:**
MW: 261.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.827E-01	25	D044	0 0 0 0 0	

1421. $C_8H_8N_2O_2$
Phthalamide
1,2-Benzenedicarboxamide
RN: 88-96-0 **MP** (°C)**:** 228
MW: 164.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-03	2.000E-01	20	A027	1 0 0 0 0	*sic*
3.594E-02	5.900E+00	30	K004	1 0 0 0 1	

1422. $C_8H_8N_2O_2$
Ricinine
Ricinin
RN: 524-40-3 **MP** (°C)**:** 201.5
MW: 164.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-02	2.700E+00	10	F300	1 0 0 0 1	

1423. $C_8H_8N_2O_3$
4-Nitroaniline-*N*-acetate
4-Nitro-anilin-*N*-acetat
p-Nitroacetanilide
1-Nitro-4-acetylaminobenzene
RN: 104-04-1 **MP** (°C)**:** 216
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
6.000E-04	1.081E-01	25	D044	0 0 0 0 0	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1424. $C_8H_8N_2O_3$
2-Nitroaniline-*N*-acetate
2-Nitro-anilin-*N*-acetat
o-Nitroacetanilide
RN: 552-32-9 **MP** (°C)**:**
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1425. $C_8H_8N_2O_6S$
MB 8882
Methyl *N*-(4-nitrobenzenesulphonyl)carbamate
RN: 3337-70-0 **MP** (°C)**:** 151
MW: 260.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.839E-03	9.990E-01	ns	M061	0 0 0 0 0	

1426. $C_8H_8N_4$
6,7-Dimethylpteridine
6:7-Dimethylpteridine
RN: 704-61-0 **MP** (°C)**:**
MW: 160.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-01	5.556E+01	20	A083	1 2 0 0 0	

1427. $C_8H_8N_4$
Hydralazine
Apresoline
RN: 86-54-4 **MP** (°C)**:** 172
MW: 160.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.996E-05	4.800E-03	22.5	B440	0 0 0 0 0	

1428. $C_8H_8N_4O$
4-Hydroxy-6,7-dimethylpteridine
4-Hydroxy-6:7-dimethylpteridine
RN: 14684-54-9 **MP** (°C)**:**
MW: 176.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.155E-03	9.083E-01	22.5	A085	1 2 0 0 0	

1429. $C_8H_8N_4O_2$
H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-oxopropyl)-
RN: 96448-61-2 **MP** (°C)**:**
MW: 192.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	3.000E-01	22	B428	1 2 1 2 1	

1430. $C_8H_8N_4O_2S_2$
2-Sulfanilamido-1,3,4-thiadiazole
Sulfathiadiazole
Sulfanilamide, *N*1-1,3,4-thiadiazol-2-yl-
RN: 16806-29-4 **MP** (°C)**:**
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.848E-03	7.300E-01	37	R045	1 2 1 1 1	

1431. $C_8H_8N_4O_3$
1-Acetoxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(acetyloxy)methyl]-1,5-dihydro-
RN: 98846-64-1 **MP** (°C)**:** 257-258
MW: 208.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	5.800E-01	22	B322	0 0 0 0 0	

1432. $C_8H_8N_4O_4$
Nifuradene
1-[5-Nitrofurfuryllidene)amino]-2-imidazolidinone
RN: 555-84-0 **MP** (°C)**:** 261.5
MW: 224.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-04	8.800E-02	ns	I310	0 0 0 0 0	

1433. $C_8H_8N_4O_4S_3$
CL 11366
RN: **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E-03	4.500E-01	ns	M032	0 0 0 0 1	

1434. $C_8H_8N_4O_4S_3$
Benzolamide
2-Benzenesulfonamide-1,3,4-thiadiazole-5-sulfonamide
5-Benzenesulfonamido-1,3,4-thiadiazole-2-sulfonamide
1,3,4-Thiadiazole-2-sulfonamide, 5-[(phenylsulfonyl)amino]-
1,3,4-Thiadiazole-2-sulfonamide, 5-benzenesulfonamido-
RN: 3368-13-6 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:** 585.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.844E-01	25	C415	1 0 0 1 0	

1435. $C_8H_8N_4O_6$
2,4,6-Trinitroethylaniline
2-4-6-Trinitromonoethylaniline
RN: 7449-27-6 **MP** (°C)**:**
MW: 256.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.904E-04	1.000E-01	19	D067	1 2 0 0 2	
1.210E-03	3.100E-01	50	D067	1 2 0 0 2	
5.699E-03	1.460E+00	100	D067	1 2 0 0 2	

1436. C_8H_8O
Acetophenone
Acetophenon
Methyl phenyl ketone
RN: 98-86-2 **MP** (°C)**:** 20.05
MW: 120.15 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.503E-02	5.411E+00	24	H106	1 0 2 2 2	
4.611E-02	5.540E+00	24	M303	1 0 1 1 2	
5.243E-02	6.300E+00	25	A003	1 2 1 2 2	
4.470E-02	5.371E+00	25	B019	1 0 1 2 0	
4.470E-02	5.371E+00	25	B092	2 1 1 1 1	
9.600E-02	1.153E+01	25	D407	1 0 2 2 2	
5.600E-03	6.729E-01	25	F063	1 1 0 0 1	
6.605E-02	7.937E+00	60	B092	2 1 1 1 1	

1437. C_8H_8O
Styrene oxide
1,2-Epoxyethylbenzene
RN: 96-09-3 **MP** (°C)**:** –36.8
MW: 120.15 **BP** (°C)**:** 194.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-02	2.792E+00	25	I313	0 0 0 0 0	

1438. C_8H_8O
2,2,3-Trimethyl-3-pentanol
2,2,3-Trimethylpentanol-3
RN: 7294-05-5 **MP** (°C)**:** –6
MW: 120.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.120E+00	4.950E+02	20	G007	1 2 0 1 2	
4.119E+00	4.949E+02	25	G007	1 2 0 1 2	
4.119E+00	4.949E+02	30	G007	1 2 0 1 2	

1439. C_8H_8O
4-Methylbenzaldehyde
p-Methylbenzaldehyde
RN: 104-87-0 **MP** (°C)**:**
MW: 120.15 **BP** (°C)**:** 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	2.271E+00	25	M017	1 2 0 1 2	

1440. $C_8H_8O_2$
2′-Hydroxyacetophenone
1-(2-Hydroxyphenyl)ethanone
2-Acetylphenol
RN: 118-93-4 **MP** (°C)**:** 6
MW: 136.15 **BP** (°C)**:** 213 at 717 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	6.808E+00	30	K441	0 0 0 0 0	
1.100E-01	1.498E+01	40	K441	0 0 0 0 0	
1.400E-01	1.906E+01	50	K441	0 0 0 0 0	

1441. $C_8H_8O_2$
4-Hydroxyacetophenone
4′-Hydroxy-acetophenon
RN: 99-93-4 **MP** (°C)**:** 110
MW: 136.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.271E-02	9.900E+00	22	F300	1 0 0 0 1	
7.000E-02	9.531E+00	30	K441	0 0 0 0 0	
1.400E-01	1.906E+01	40	K441	0 0 0 0 0	
1.800E-01	2.451E+01	50	K441	0 0 0 0 0	

1442. $C_8H_8O_2$
p-Anisaldehyde
Anisaldehyd
p-Methoxybenzaldehyde
RN: 123-11-5 **MP** (°C)**:** 0
MW: 136.15 **BP** (°C)**:** 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-02	2.000E+00	20	F300	1 0 0 0 0	
3.900E-02	5.310E+00	25	D407	1 0 2 2 2	
3.150E-02	4.289E+00	25	I019	1 0 1 2 2	

1443. $C_8H_8O_2$
m-Toluic acid
3-Methylbenzoic acid
m-Methylbenzoic acid
β-Methylbenzoic acid
RN: 99-04-7 **MP** (°C)**:** 112
MW: 136.15 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	9.803E-01	25	F001	1 0 1 0 2	
7.198E-03	9.800E-01	25	F300	1 0 0 0 2	
7.785E-03	1.060E+00	37	M360	1 2 1 1 2	

1444. $C_8H_8O_2$
p-Toluic acid
4-Methylbenzoic acid
Toluenecarboxylic acid
RN: 99-94-5 **MP** (°C)**:** 180
MW: 136.15 **BP** (°C)**:** 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	3.404E-01	25	F001	1 0 1 0 2	
2.938E-03	4.000E-01	25	F300	1 0 0 0 2	
2.277E-03	3.100E-01	37	M360	1 2 1 1 2	
2.780E-03	3.785E-01	ns	C014	0 0 0 1 2	

1445. $C_8H_8O_2$
o-Toluic acid
o-Tolylsaeure
o-Toluylic acid
2-Methylbenzoic acid
RN: 118-90-1 **MP** (°C)**:** 107
MW: 136.15 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-03	1.185E+00	25	F001	1 0 1 0 2	
8.780E-03	1.195E+00	25	R016	0 0 0 0 0	
1.014E-02	1.380E+00	37	M360	1 2 1 1 2	

1446. $C_8H_8O_2$
Phenylacetic acid
Phenylessigsaeure
RN: 103-82-2 **MP** (°C)**:** 76.5
MW: 136.15 **BP** (°C)**:** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-01	1.600E+01	20	F071	1 1 2 1 2	
1.219E-01	1.660E+01	20	H080	1 0 0 0 2	
1.219E-01	1.660E+01	20	M344	1 0 0 0 2	
1.300E-01	1.770E+01	25	F300	1 0 0 0 2	
1.267E-01	1.725E+01	25	H071	2 2 2 1 2	
1.310E-01	1.784E+01	25	K040	1 0 2 1 2	
1.300E-01	1.770E+01	25.00	M135	1 2 1 1 2	0.01N sodium phenylacetate
1.451E-01	1.975E+01	30	D033	2 2 1 2 2	
1.910E-01	2.600E+01	35.00	M135	1 2 1 1 2	
2.113E-01	2.877E+01	40	D033	2 2 1 2 2	
2.880E-01	3.921E+01	41.50	M135	1 2 1 1 2	
2.900E-01	3.948E+01	45.00	M135	1 2 1 1 2	
3.650E-01	4.970E+01	58.40	M135	1 2 1 1 2	

(*continued*)

1446. $C_8H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-01	5.923E+01	68.80	M135	1 2 1 1 2	
5.130E-01	6.985E+01	76.50	M135	1 2 1 1 2	
6.110E-01	8.319E+01	83.00	M135	1 2 1 1 2	
6.860E-01	9.340E+01	86.70	M135	1 2 1 1 2	
7.712E-01	1.050E+02	100	F300	1 0 0 0 2	
1.259E-01	1.714E+01	ns	R424	0 0 0 0 0	

1447. $C_8H_8O_2$

Methyl benzoate
Methyl *p*-hydroxybenzoate

RN: 93-58-3 **MP** (°C)**:** –12
MW: 136.15 **BP** (°C)**:** 198

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.337E-03	9.990E-01	15	G040	1 0 2 0 0	
3.085E-02	4.200E+00	22	N317	1 1 2 1 2	
2.926E-02	3.984E+00	25	G040	1 0 2 0 0	
1.447E-02	1.970E+00	25	L086	1 0 1 1 2	
1.497E-02	2.038E+00	25	M334	1 0 1 1 2	
1.777E-02	2.420E+00	30	L012	2 0 2 2 2	
1.796E-02	2.445E+00	30	L086	1 0 1 1 2	
3.654E-02	4.975E+00	35	G040	1 0 2 0 0	
2.221E-02	3.024E+00	35	L086	1 0 1 1 2	
2.723E-02	3.708E+00	40	L086	1 0 1 1 2	

1448. $C_8H_8O_2Hg$

Phenylmercuric acetate
Ceresan
PMAC
Acetate, phenylmercuric
PMA

RN: 62-38-4 **MP** (°C)**:** 149
MW: 336.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-02	2.470E+01	20	M061	1 0 0 0 2	
1.389E-02	4.678E+00	ns	B185	0 0 0 0 0	
1.396E-02	4.700E+00	ns	N013	0 0 0 0 2	
1.298E-02	4.370E+00	rt	M161	0 0 0 0 2	

1449. $C_8H_8O_3$
Methyl salicylate
Salicylsaeure-methyl ester
Methyl hydroxybenzoate
Betula oil
Panalgesic
Betula
RN: 119-36-8 **MP** (°C)**:** –8
MW: 152.15 **BP** (°C)**:** 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.206E-03	6.400E-01	21	B331	0 0 0 0 0	
4.000E-03	6.086E-01	25	D407	1 0 2 2 2	
1.312E-02	1.996E+00	25	R041	0 0 0 0 0	
4.601E-03	7.000E-01	30	F300	1 0 0 0 0	
6.244E-03	9.500E-01	30	L012	2 0 2 2 1	

1450. $C_8H_8O_3$
Vanillin
4-Hydroxy-3-methoxybenzaldehyde
3-Methoxy-4-hydroxybenzaldehyde
Methylprotocatechuic aldehyde
Vanillic aldehyde
Vanillaldehyde
RN: 121-33-5 **MP** (°C)**:** 82
MW: 152.15 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-02	6.754E+00	.2	D073	1 1 2 1 1	
1.972E-02	3.000E+00	4.40	M096	1 1 2 1 1	
3.418E-02	5.200E+00	15.60	M096	1 1 2 1 2	
8.114E-02	1.235E+01	20	D073	1 1 2 1 2	
6.572E-02	1.000E+01	20	F300	1 0 0 0 0	
5.915E-02	9.000E+00	23.90	M096	1 1 2 1 2	
4.800E-02	7.303E+00	25	D407	1 0 2 2 2	
7.240E-02	1.102E+01	25	I019	1 0 1 2 2	
9.713E-02	1.478E+01	30	D073	1 1 2 1 2	
8.500E-02	1.293E+01	30	L069	1 0 1 1 0	EFG
1.697E-01	2.582E+01	40	D073	1 1 2 1 2	
3.010E-01	4.580E+01	50	D073	1 1 2 1 2	
3.160E-01	4.807E+01	60	D073	1 1 2 1 2	
3.286E-01	5.000E+01	80	F300	1 0 0 0 0	

1451. $C_8H_8O_3$

Methylparaben
Me-paraben
Methyl *p*-hydroxybenzoic acid
Methyl 4-hydroxybenzoate
Methyl paraben

RN: 99-76-3 **MP** (°C)**:** 131
MW: 152.15 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.310E-03	1.264E+00	15	B355	0 0 0 0 0	
1.026E-02	1.561E+00	15	M352	1 1 1 1 2	
9.970E-03	1.517E+00	20	B355	0 0 0 0 0	
1.334E-02	2.030E+00	20	H056	1 0 2 1 2	
1.441E-02	2.193E+00	25	A059	1 0 1 1 2	
1.140E-02	1.735E+00	25	B355	0 0 0 0 0	
1.639E-02	2.494E+00	25	D081	1 2 2 1 2	
1.600E-02	2.434E+00	25	D339	0 0 0 0 0	
3.162E-02	4.811E+00	25	F322	2 0 1 1 0	EFG
1.364E-02	2.075E+00	25	L075	1 0 1 1 2	
1.393E-02	2.120E+00	25	L338	1 0 1 1 2	
1.460E-02	2.221E+00	25	M014	2 0 1 1 2	
1.585E-02	2.412E+00	25	M352	1 1 1 1 2	
1.643E-02	2.500E+00	25	O027	1 0 1 0 1	
1.485E-02	2.260E+00	25	P013	0 0 0 0 0	
1.446E-02	2.200E+00	25	P053	1 0 1 1 2	
1.600E-02	2.434E+00	27	B129	2 2 2 2 2	
1.500E-02	2.282E+00	27	G078	2 1 0 1 0	EFG
1.600E-02	2.434E+00	27	P019	1 2 1 1 0	EFG
1.450E-02	2.206E+00	27.0	G067	2 0 1 1 2	
1.828E-02	2.782E+00	30	A059	1 0 1 1 2	
1.564E-02	2.380E+00	30	M325	1 0 0 0 1	
2.275E-02	3.462E+00	35	A059	1 0 1 1 2	
2.550E-02	3.880E+00	37	B171	2 0 1 1 2	
2.268E-02	3.451E+00	39.3	G302	2 2 2 2 0	EFG
2.551E-02	3.882E+00	40	A059	1 0 1 1 2	
3.773E-02	5.740E+00	40	M352	1 1 1 1 2	
4.168E-02	6.341E+00	50	M352	1 1 1 1 2	

1452. $C_8H_8O_3$

D-Mandelic acid
(*R*)(–)Mandelic acid
(*S*)-α-Hydroxybenzeneacetic acid
L-Mandelic acid
(*S*)-(+)-Mandelic acid

RN: 17199-29-0 **MP** (°C)**:** 132
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.310E-01	8.080E+01	0	A043	1 2 1 1 2	
5.310E-01	8.080E+01	0	L035	1 2 2 1 2	

(*continued*)

1452. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-01	1.046E+02	10	A043	1 2 1 1 2	
6.874E-01	1.046E+02	10	L035	1 2 2 1 2	
7.766E-01	1.182E+02	15	A043	1 2 1 1 2	
7.766E-01	1.182E+02	15	L035	1 2 2 1 2	
9.158E-01	1.393E+02	20	A043	1 2 1 1 2	
9.158E-01	1.393E+02	20	L035	1 2 2 1 2	
5.371E-01	8.173E+01	24.5	L035	1 2 2 1 1	
5.371E-01	8.173E+01	24.50	A043	1 2 1 1 1	
1.183E+00	1.800E+02	25	A043	1 2 1 1 2	
6.503E-01	9.894E+01	25	C045	2 2 0 1 2	
6.705E-01	1.020E+02	25	C045	2 2 0 1 2	
1.183E+00	1.800E+02	25	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.5	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.50	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.5	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.50	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	L035	1 2 2 1 2	
3.434E+00	5.224E+02	37	A043	1 2 1 1 2	
1.132E+00	1.722E+02	37	A043	1 2 1 1 2	
3.434E+00	5.224E+02	37	L035	1 2 2 1 2	
1.132E+00	1.722E+02	37	L035	1 2 2 1 2	
4.075E+00	6.201E+02	40	A043	1 2 1 1 2	
4.075E+00	6.201E+02	40	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.5	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.50	A043	1 2 1 1 2	
4.325E+00	6.580E+02	42.5	L035	1 2 2 1 2	
4.325E+00	6.580E+02	42.50	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45.50	A043	1 2 1 1 2	
2.351E+00	3.577E+02	46.5	L035	1 2 2 1 2	
2.351E+00	3.577E+02	46.50	A043	1 2 1 1 2	
4.816E+00	7.328E+02	47	L035	1 2 2 1 2	
4.816E+00	7.328E+02	47.50	A043	1 2 1 1 2	
2.795E+00	4.253E+02	48.5	L035	1 2 2 1 2	
2.795E+00	4.253E+02	48.50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.5	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.50	A043	1 2 1 1 2	
3.484E+00	5.301E+02	52.5	L035	1 2 2 1 2	
3.484E+00	5.301E+02	52.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	L035	1 2 2 1 2	
3.996E+00	6.080E+02	57	A043	1 2 1 1 2	

(*continued*)

1452. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.996E+00	6.080E+02	57	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.5	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.50	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	L035	1 2 2 1 2	

1453. $C_8H_8O_3$

m-Cresotic acid
2-Hydroxy-*p*-tolylsaeure-(1)
m-Kresotinsaeure

RN: 50-85-1 **MP** (°C)**:** 177
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.638E-02	1.010E+01	100	F300	1 0 0 0 2	

1454. $C_8H_8O_3$

o-Anisic acid
2-Methoxybenzoic acid
Salicylic acid methyl ether
Salicylsaeure-methylaether
o-Methoxybenzoic acid

RN: 579-75-9 **MP** (°C)**:** 101
MW: 152.15 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-02	1.567E+00	4.99	A405	2 0 1 1 2	
1.220E-02	1.856E+00	9.99	A405	2 0 1 1 2	
1.420E-02	2.161E+00	14.99	A405	2 0 1 1 2	
1.710E-02	2.602E+00	19.99	A405	2 0 1 1 2	
2.070E-02	3.150E+00	23.99	A405	2 0 1 1 2	
2.760E-02	4.200E+00	25	H007	0 0 0 0 0	
2.440E-02	3.712E+00	26.99	A405	2 0 1 1 2	
3.286E-02	5.000E+00	30	F300	1 0 0 0 0	
2.760E-02	4.199E+00	30.99	A405	2 0 1 1 2	
3.120E-02	4.747E+00	34.99	A405	2 0 1 1 2	
3.503E-02	5.330E+00	37	M360	1 2 1 1 2	
3.750E-02	5.706E+00	38.99	A405	2 0 1 1 2	
4.390E-02	6.679E+00	41.99	A405	2 0 1 1 2	
4.800E-02	7.303E+00	44.99	A405	2 0 1 1 2	
5.930E-02	9.023E+00	47.99	A405	2 0 1 1 2	
6.930E-02	1.054E+01	52.99	A405	2 0 1 1 2	
8.370E-02	1.274E+01	53.99	A405	2 0 1 1 2	
9.500E-02	1.445E+01	56.99	A405	2 0 1 1 2	
1.261E-01	1.919E+01	60.99	A405	2 0 1 1 2	
1.683E-01	2.561E+01	64.99	A405	2 0 1 1 2	

(*continued*)

1454. $C_8H_8O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.326E-01	3.539E+01	68.99	A405	2 0 1 1 2	
2.630E-01	4.002E+01	69.99	A405	2 0 1 1 2	
3.467E-01	5.275E+01	72.99	A405	2 0 1 1 2	

1455. $C_8H_8O_3$
Mandelic acid
Amygdalic acid
α-Hydroxyphenylacetic acid
Uromaline
α-Hydroxy-benzeneacetic acid
RN: 90-64-2 **MP** (°C)**:** 119.0
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.191E+00	1.812E+02	25	K040	1 0 2 1 2	*sic*
8.795E-03	1.338E+00	25	R049	0 0 0 0 0	
9.120E-01	1.388E+02	ns	R427	0 0 0 0 0	

1456. $C_8H_8O_3$
3-Hydroxy-*p*-toluic acid
3-Hydroxy-*p*-tolylsaeure-(1)
RN: 586-30-1 **MP** (°C)**:**
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.859E-01	4.350E+01	100	F300	1 0 0 0 2	

1457. $C_8H_8O_3$
3-Methoxybenzoic acid
3-Methoxy-benzoesaeure
m-Anisic acid
m-Methoxybenzoic acid
RN: 586-38-9 **MP** (°C)**:** 110
MW: 152.15 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.282E-02	1.950E+00	37	M360	1 2 1 1 2	
1.183E-03	1.800E-01	ns	B361	0 0 0 0 0	

1458. $C_8H_8O_3$
DL-Mandelic acid
DL-Mandelsaeure
RN: 611-72-3 **MP** (°C)**:** 122
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.050E-01	1.377E+02	20	F300	1 0 0 0 2	
1.134E+00	1.725E+02	24	F300	1 0 0 0 2	

1459. $C_8H_8O_3$
4-Hydroxy-*m*-toluic acid
4-Hydroxy-*m*-tolylsaeure-(1)
o-Cresotic acid
2-Hydroxy-*m*-toluic acid
2-Hydroxy-*m*-tolylsaeure-(1)
RN: 83-40-9 **MP** (°C)**:** 165.5
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-02	1.160E+01	100	F300	1 0 0 0 2	
3.411E-01	5.190E+01	100	F300	1 0 0 0 2	

1460. $C_8H_8O_3$
Phenoxyacetic acid
Glycolic acid phenyl ether
O-Phenylglycolic acid
RN: 122-59-8 **MP** (°C)**:** 98
MW: 152.15 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.887E-02	1.200E+01	10	F071	1 1 2 1 2	
8.084E-03	1.230E+00	10	F300	1 0 0 0 2	
7.887E-02	1.200E+01	10	H080	1 0 0 0 2	
7.887E-02	1.200E+01	10	M344	1 0 0 0 2	
1.100E-04	1.674E-02	25	L030	1 0 2 1 2	

1461. $C_8H_8O_3$
p-Methoxybenzoic acid
4-Methoxybenzoic acid
p-Anisic acid
Anissaeure
RN: 100-09-4 **MP** (°C)**:** 184
MW: 152.15 **BP** (°C)**:** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.111E-01	2.99	A405	2 0 1 1 2	
9.400E-04	1.430E-01	4.99	A405	2 0 1 1 2	
1.070E-03	1.628E-01	10.99	A405	2 0 1 1 2	
1.270E-03	1.932E-01	14.99	A405	2 0 1 1 2	
1.775E-02	2.700E+00	19	F300	1 0 0 0 1	
1.330E-03	2.024E-01	19.99	A405	2 0 1 1 2	
1.680E-03	2.556E-01	24.99	A405	2 0 1 1 2	
2.020E-03	3.073E-01	28.99	A405	2 0 1 1 2	
2.300E-03	3.499E-01	33.99	A405	2 0 1 1 2	
3.483E-03	5.300E-01	37	B171	2 0 1 1 2	
1.380E-03	2.100E-01	37	M360	1 2 1 1 2	
3.110E-03	4.732E-01	39.99	A405	2 0 1 1 2	
3.870E-03	5.888E-01	43.99	A405	2 0 1 1 2	
5.130E-03	7.805E-01	50.99	A405	2 0 1 1 2	
6.110E-03	9.296E-01	55.99	A405	2 0 1 1 2	
8.170E-03	1.243E+00	59.99	A405	2 0 1 1 2	
9.000E-03	1.369E+00	64.99	A405	2 0 1 1 2	
1.080E-02	1.643E+00	65.99	A405	2 0 1 1 2	
1.100E-02	1.674E+00	66.99	A405	2 0 1 1 2	
1.460E-02	2.221E+00	71.99	A405	2 0 1 1 2	
1.778E-02	2.706E+00	ns	R427	0 0 0 0 0	

1462. $C_8H_8O_3$
p-Cresotic acid
6-Hydroxy-*m*-toluic acid
6-Hydroxy-*m*-tolylsaeure-(1)
RN: 89-56-5 **MP** (°C)**:** 151
MW: 152.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	2.190E+01	100	F300	1 0 0 0 2	

1463. $C_8H_8O_4$
Vanillic acid
Vanillinsaeure
RN: 121-34-6 **MP** (°C)**:** 214
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.921E-03	1.500E+00	14	F300	1 0 0 0 1	
1.546E-01	2.600E+01	100	F300	1 0 0 0 2	

1464. $C_8H_8O_4$
Homogentisic acid
2,5-Dihydroxyphenylacetic acid
2,5-Dihydroxy-benzeneacetic acid
RN: 451-13-8 **MP** (°C)**:** 151
MW: 168.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.732E+00	4.595E+02	25	D041	1 0 0 0 1	

1465. $C_8H_8O_5$
Methyl gallate
Gallussaeuremethyl ester
Methyl-3,4,5-trihydroxybenzoate
RN: 99-24-1 **MP** (°C)**:** 201.5
MW: 184.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.323E-02	9.803E+00	19.99	L430	0 0 0 0 0	
5.696E-02	1.049E+01	24.99	L430	0 0 0 0 0	
6.757E-02	1.244E+01	29.99	L430	0 0 0 0 0	
9.549E-02	1.759E+01	34.99	L430	0 0 0 0 0	
1.340E-01	2.468E+01	39.99	L430	0 0 0 0 0	
1.704E-01	3.138E+01	44.99	L430	0 0 0 0 0	
2.542E-01	4.680E+01	49.99	L430	0 0 0 0 0	
4.328E-01	7.970E+01	54.99	L430	0 0 0 0 0	
5.879E-01	1.083E+02	59.99	L430	0 0 0 0 0	
7.775E-01	1.432E+02	64.99	L430	0 0 0 0 0	
1.054E+00	1.941E+02	69.99	L430	0 0 0 0 0	
1.624E-02	2.991E+00	–.0	L430	0 0 0 0 0	
5.756E-02	1.060E+01	ns	F300	0 0 0 0 2	

1466. $C_8H_9ClNO_5PS$

Chlorthion
O,O-Dimethyl *O*-4-nitro-3-chlorophenyl thiophosphate
RN: 500-28-7 **MP** (°C)**:** 21
MW: 297.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.344E-04	4.000E-02	20	M061	1 0 0 0 1	

1467. $C_8H_9ClNO_5PS$

Dicapthon
O-(2-Chloro-4-nitrophenyl) *O,O*-dimethyl phosphorothioate
Dicaptan
Isochlorthion
RN: 2463-84-5 **MP** (°C)**:**
MW: 297.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B300	2 1 1 1 2	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
2.100E-05	6.250E-03	20	C053	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
2.100E-05	6.250E-03	ns	F071	0 1 2 1 2	
1.176E-04	3.500E-02	ns	M061	0 0 0 0 1	
2.620E-05	7.800E-03	rt	F040	1 2 2 2 1	

1468. C_8H_9ClO

2,5-Dimethyl-4-chloro-phenol
4-Chloro-2,5-xylenol
4-Chloro-2,5-dimethylphenol
RN: 1124-06-7 **MP** (°C)**:** 114–116
MW: 156.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	8.927E+00	25	B316	0 0 0 0 0	

1469. C_8H_9ClO

2,6-Dimethyl-4-chloro-phenol
4-Chloro-2,6-xylenol
RN: 1123-63-3 **MP** (°C)**:**
MW: 156.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-03	5.168E-01	25	B316	0 0 0 0 0	

1470. C_8H_9ClO
Chloroxylenol
3,5-Dimethyl-4-chloro-phenol-
RN: 88-04-0 **MP** (°C)**:** 115.5
MW: 156.61 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	2.500E-01	20	M018	1 2 2 1 0	EFG
1.979E-03	3.099E-01	20	M093	1 0 0 1 1	
2.200E-02	3.445E+00	25	B316	0 0 0 0 0	*sic*
1.915E-03	2.999E-01	25	R041	0 0 0 0 0	
1.585E-03	2.482E-01	ns	R427	0 0 0 0 0	

1471. $C_8H_9FN_2O_3$
2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxobutyl)-
RN: 94452-21-8 **MP** (°C)**:**
MW: 200.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-02	1.061E+01	22	B416	2 2 1 2 1	

1472. $C_8H_9FN_2O_3$
Ftorafur
THFFU
1-(2-Tetrahydrofuryl)-5-fluorouracil
RN: 37076-68-9 **MP** (°C)**:** 167
MW: 200.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	2.802E+01	37	N017	0 0 0 0 0	

1473. $C_8H_9FN_2O_4$
1-Propionyloxymethyl-5-fluorouracil
1-Propionyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
RN: 66542-36-7 **MP** (°C)**:** 100–102
MW: 216.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-01	3.360E+01	22	B321	0 0 0 0 0	pH 4.0

1474. $C_8H_9FN_2O_4$
1-Isopropyloxyarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 1-methylethyl ester
RN: 109232-73-7 **MP** (°C)**:** 180
MW: 216.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E-02	4.700E+00	22	B332	1 1 0 0 1	pH 4.0

1475. C_8H_9N
Indoline
2,3-Dihydro-1H-indole
2,3-Dihydroindole
RN: 496-15-1 **MP** (°C)**:** <25
MW: 119.17 **BP** (°C)**:** 220.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.934E-02	3.497E+00	20.3	L339	2 0 2 2 2	
9.063E-02	1.080E+01	25	P051	2 1 1 2 2	
9.063E-02	1.080E+01	25.00	P007	2 1 2 2 1	
3.651E-02	4.350E+00	40.0	L339	2 0 2 2 2	
4.586E-02	5.465E+00	59.4	L339	2 0 2 2 2	
5.738E-02	6.838E+00	79.0	L339	2 0 2 2 2	
8.142E-02	9.703E+00	100.0	L339	2 0 2 2 2	

1476. C_8H_9NO
p-Aminoacetophenone
4′-Aminoacetophenone
RN: 99-92-3 **MP** (°C)**:** 106
MW: 135.17 **BP** (°C)**:** 294

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.480E-02	3.352E+00	37.5	G002	1 1 1 1 2	

1477. C_8H_9NO
Acetanilide
Acetanilid
RN: 103-84-4 **MP** (°C)**:** 114
MW: 135.17 **BP** (°C)**:** 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.652E-02	3.585E+00	0	L029	2 2 2 2 2	
3.534E-02	4.777E+00	10	M043	1 0 0 0 1	
3.251E-02	4.395E+00	10.1	L029	2 2 2 2 2	
2.970E-02	4.014E+00	14	O016	1 0 0 0 2	
3.688E-02	4.985E+00	15	L038	1 0 1 0 2	

(*continued*)

1477. C_8H_9NO (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-02	5.015E+00	20	B101	0 0 0 0 0	
3.666E-02	4.955E+00	20	K078	1 0 2 1 2	
4.129E-02	5.581E+00	20	L029	2 2 2 2 2	
3.827E-02	5.173E+00	20	M043	1 0 0 0 1	
3.330E-02	4.501E+00	20	O019	1 0 0 1 2	
3.884E-02	5.250E+00	20	W026	1 0 1 1 1	average of 2
4.142E-02	5.598E+00	25	B101	0 0 0 0 0	
4.450E-02	6.015E+00	25	B434	0 0 0 0 0	
4.786E-02	6.468E+00	25	B434	0 0 0 0 0	
4.160E-02	5.623E+00	25	D044	0 0 0 0 0	
4.143E-02	5.600E+00	25	F300	1 0 0 0 1	
4.697E-02	6.349E+00	25	L029	2 2 2 2 2	
4.486E-02	6.063E+00	25	M094	1 0 0 1 1	
3.699E-02	5.000E+00	25	P016	1 0 0 1 0	
4.887E-02	6.606E+00	30	B101	0 0 0 0 0	
5.262E-02	7.113E+00	30	B434	0 0 0 0 0	
5.240E-02	7.083E+00	30	B434	0 0 0 0 0	
5.351E-02	7.232E+00	30	L029	2 2 2 2 2	
4.632E-02	6.261E+00	30	M043	1 0 0 0 1	
5.253E-02	7.100E+00	30	W026	1 0 1 1 1	average of 2
5.792E-02	7.828E+00	32.6	L038	1 0 1 0 2	
5.930E-02	8.015E+00	35	B101	0 0 0 0 0	
5.799E-02	7.838E+00	35	B434	0 0 0 0 0	
5.760E-02	7.786E+00	35	B434	0 0 0 0 0	
6.787E-02	9.174E+00	40	B434	0 0 0 0 0	
6.730E-02	9.097E+00	40	B434	0 0 0 0 0	
7.134E-02	9.643E+00	40	L029	2 2 2 2 2	
6.381E-02	8.625E+00	40	M043	1 0 0 0 1	
9.682E-02	1.309E+01	50	L029	2 2 2 2 2	
1.349E-01	1.823E+01	60	L029	2 2 2 2 2	
1.522E-01	2.057E+01	60	M043	1 0 0 0 1	
1.928E-01	2.606E+01	70	L029	2 2 2 2 2	
3.321E-01	4.489E+01	80	M043	1 0 0 0 1	
4.047E-02	5.470E+00	rt	D021	0 0 1 1 1	

1478. C_8H_9NO

m-Aminoacetophenone
3′-Aminoacetophenone

RN: 99-03-6 **MP** (°C)**:** 97
MW: 135.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.220E-02	7.056E+00	37.5	G002	1 1 1 1 2	pH 6.8

1479. $C_8H_9NO_2$
Acetaminophen
4-Acetamidophenol
4-Amino-phenol-*N*-acetat
p-Acetaminophen
p-Hydroxyacetanilide
RN: 103-90-2 **MP** (°C)**:** 167
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.307E-02	1.105E+01	15	M352	1 1 1 1 2	
5.462E-01	8.257E+01	16.9	Y412	0 0 0 0 0	
6.014E-01	9.091E+01	21.5	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	25	B010	1 1 1 1 0	
1.016E-01	1.536E+01	25	B434	0 0 0 0 0	
9.500E-02	1.436E+01	25	C032	2 2 1 2 0	EFG
7.710E-02	1.165E+01	25	D044	0 0 0 0 0	
9.133E-02	1.381E+01	25	D078	1 2 1 1 2	
5.185E-02	7.838E+00	25	F415	0 0 0 0 0	Average
1.000E-01	1.512E+01	25	K041	1 0 0 0 0	
9.851E-02	1.489E+01	25	M352	1 1 1 1 2	
9.923E-02	1.500E+01	25	P016	1 0 0 1 1	
7.277E-02	1.100E+01	25	P312	0 0 0 0 0	
9.326E-02	1.410E+01	25	W019	1 0 1 1 2	
3.538E-01	5.348E+01	25	Y410	0 0 0 0 0	
9.140E-02	1.382E+01	25	Z408	0 0 0 0 0	
6.556E-01	9.910E+01	26.3	Y412	0 0 0 0 0	
1.241E-01	1.876E+01	30	B434	0 0 0 0 0	
1.240E-01	1.874E+01	30	B434	0 0 0 0 0	
1.120E-01	1.693E+01	30	L069	1 0 1 1 0	EFG
7.088E-01	1.071E+02	31.5	Y412	0 0 0 0 0	
1.684E-01	2.545E+01	35	B434	0 0 0 0 0	
1.684E-01	2.546E+01	35	B434	0 0 0 0 0	
7.610E-01	1.150E+02	35.3	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	37	F076	2 0 2 2 0	
1.442E-01	2.180E+01	37	K086	1 0 0 0 2	
8.124E-01	1.228E+02	37	Y412	0 0 0 0 0	
1.349E-01	2.039E+01	39.3	G302	2 0 2 2 0	EFG
2.234E-01	3.377E+01	40	B434	0 0 0 0 0	
2.238E-01	3.384E+01	40	B434	0 0 0 0 0	
1.440E-01	2.177E+01	40	M352	1 1 1 1 2	
1.800E-01	2.720E+01	50	M352	1 1 1 1 2	
1.019E-01	1.540E+01	c	B434	0 0 0 0 0	
6.615E-04	1.000E-01	ns	K444	0 0 0 0 0	
8.004E-02	1.210E+01	rt	R431	0 0 0 0 0	Average

1480. $C_8H_9NO_2$
Benzyl carbamate
O-Benzyl carbamate
Benzyloxycarbonyl amine
RN: 621-84-1 **MP** (°C)**:** 87
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-01	6.802E+01	37	H006	1 2 2 1 1	
4.467E-01	6.752E+01	ns	R427	0 0 0 0 0	

1481. $C_8H_9NO_2$
DL-2-Phenylglycine
2-Amino-phenyl-essigsaeure
2-Aminophenylacetic acid
RN: 2835-06-5 **MP** (°C)**:** 255
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.608E-01	1.150E+02	100	F300	1 0 0 0 2	

1482. $C_8H_9NO_2$
N-Methylanthranilic acid
N-Methyl-anthranilsaeure
RN: 119-68-6 **MP** (°C)**:** 171
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-03	2.000E-01	20	F300	1 0 0 0 2	
2.646E-03	4.000E-01	100	F300	1 0 0 0 2	

1483. $C_8H_9NO_2$
D-Phenylglycine
D-2-Phenylglycine
D-(–)-α-Aminophenylacetic acid
Benzeneacetic acid, α-amino-
RN: 875-74-1 **MP** (°C)**:** 302 C
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-02	4.586E+00	25	R419	0 0 0 0 0	

1484. $C_8H_9NO_2$

Methyl-*p*-aminobenzoate
Methyl *p*-aminobenzoate
4-Aminobenzoic acid methyl ester
RN: 619-45-4 **MP** (°C)**:**
MW: 151.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.884E-03	8.894E-01	15	M352	1 1 1 1 2	
9.542E-03	1.442E+00	25	M352	1 1 1 1 2	
1.070E-02	1.618E+00	25	P303	0 0 0 0 0	
1.397E-02	2.112E+00	33	P303	0 0 0 0 0	
2.530E-02	3.825E+00	37	F006	1 1 2 2 2	
1.646E-02	2.488E+00	40	M352	1 1 1 1 2	
1.839E-02	2.780E+00	40	P303	0 0 0 0 0	
7.940E-03	1.200E+00	ns	M066	0 0 0 0 2	
7.940E-03	1.200E+00	rt	B016	0 0 1 1 2	pH 7.4

1485. $C_8H_9NO_2S_2$

2-(2-Thienyl)-L-thiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-(2-thienyl)-
RN: 32451-19-7 **MP** (°C)**:**
MW: 215.29 **BP** (°C)**:** 454.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.055E+00	21	B414	1 0 0 1 1	fast decomposition

1486. $C_8H_9NO_3$

D-(*p*-hydroxy)phenylglycine
RN: **MP** (°C)**:**
MW: 167.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-01	1.937E+01	25	R419	0 0 0 0 0	

1487. $C_8H_9NO_3S$

p-Acetylbenzenesulfonamide
4-Acetylbenzenesulfonamide
RN: 1565-17-9 **MP** (°C)**:**
MW: 199.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.582E-01	15	K024	1 2 1 1 2	

1488. $C_8H_9NO_4$
Biliverdic acid
Biliverdinsaeure
RN: 487-65-0 **MP** (°C)**:**
MW: 183.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-01	3.900E+01	20	F300	1 0 0 0 1	

1489. $C_8H_9N_3O_3$
Orotic acid allylamide
4-Pyrimidinecarboxamide, 1,2,3,6-tetrahydro-2,6-dioxo-*N*-2-propenyl-
RN: 292870-71-4 **MP** (°C)**:** 259–262
MW: 195.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-01	3.474E+01	−4	N018	0 0 0 0 0	
3.000E-01	5.855E+01	16	N018	0 0 0 0 0	
3.710E-01	7.241E+01	25	N018	0 0 0 0 0	

1490. $C_8H_9N_5$
7-Dimethylaminopteridine
7-Pteridinamine, *N,N*-dimethyl-
RN: 204443-26-5 **MP** (°C)**:**
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.154E-01	1.429E+02	20	A083	1 2 0 0 0	
1.903E+00	3.333E+02	100	A083	1 2 0 0 0	

1491. $C_8H_9N_5$
2-Dimethylaminopteridine
2-Pteridinamine, *N,N*-dimethyl-
RN: 41047-52-3 **MP** (°C)**:**
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.631E+00	2.857E+02	22.5	A085	1 2 0 0 0	

1492. $C_8H_9N_5$
4-Dimethylaminopteridine
4-Pteridinamine, *N,N*-dimethyl-
RN: 14131-04-5 **MP** (°C)**:** 165
MW: 175.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.357E-02	1.639E+01	20	A019	2 2 1 1 0	
1.392E-01	2.439E+01	100	A019	1 2 1 1 0	

1493. $C_8H_9O_3PS$
2-Methoxy-4H-benzo-1,3,2-dioxaphosphorin-2-thione
Dioxabenzofos
Salithion
Fenfosphorin
Dioxabenzophos
RN: 3811-49-2 **MP** (°C)**:** 55.5
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-04	5.800E-02	30	M161	1 0 0 0 1	

1494. C_8H_{10}
Ethylbenzene
Phenylethane
Ethylenzene
Ethylbenzol
EB
RN: 100-41-4 **MP** (°C)**:** –95
MW: 106.17 **BP** (°C)**:** 136.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.856E-03	1.970E-01	0	P003	2 2 2 2 2	
1.846E-03	1.960E-01	4.50	B086	2 1 2 2 2	
1.808E-03	1.920E-01	6.30	B086	2 1 2 2 2	
1.677E-03	1.781E-01	7.09	F418	0 0 0 0 0	
1.752E-03	1.860E-01	7.10	B086	2 1 2 2 2	
1.761E-03	1.870E-01	9	B086	2 1 2 2 2	
1.910E-03	2.028E-01	10	B149	2 1 1 2 2	
1.850E-03	1.964E-01	10	O312	2 2 0 2 2	
1.705E-03	1.810E-01	11.80	B086	2 1 2 2 2	
1.723E-03	1.830E-01	12.10	B086	2 1 2 2 2	
1.812E-03	1.924E-01	14	O312	2 2 0 2 2	
1.300E-03	1.380E-01	15	F001	1 0 1 2 1	
1.300E-03	1.380E-01	15	S006	1 0 0 0 1	
1.658E-03	1.760E-01	15	S203	1 1 2 1 2	
1.695E-03	1.800E-01	15.10	B086	2 1 2 2 2	

(*continued*)

1494. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.639E-03	1.740E-01	16.93	F418	0 0 0 0 0	
1.776E-03	1.886E-01	17	O312	2 2 0 2 2	
1.733E-03	1.840E-01	17.90	B086	2 1 2 2 2	
2.901E-03	3.080E-01	18	F185	1 0 0 0 2	
2.788E-03	2.960E-01	18	F185	1 0 0 0 2	
1.725E-03	1.831E-01	18	O312	2 2 0 2 2	
3.080E-03	3.270E-01	19	F185	1 0 0 0 2	
1.676E-03	1.779E-01	19	O312	2 2 0 2 2	
2.000E-03	2.123E-01	20	B149	2 1 1 2 2	
1.695E-03	1.800E-01	20	B356	0 0 0 0 0	
1.770E-03	1.879E-01	20	O312	2 2 0 2 2	
1.695E-03	1.800E-01	20.10	B086	2 1 2 2 1	
1.724E-03	1.830E-01	21	O312	2 2 0 2 2	
3.297E-03	3.500E-01	22	F185	1 0 0 0 2	
1.713E-03	1.819E-01	22	O312	2 2 0 2 2	
3.391E-03	3.600E-01	23	F185	1 0 0 0 2	
1.751E-03	1.859E-01	23.5	O312	2 2 0 2 2	
3.655E-03	3.880E-01	24	F185	1 0 0 0 2	
1.582E-03	1.680E-01	25	A002	1 2 1 1 2	
1.883E-03	2.000E-01	25	A094	1 0 0 0 0	
1.959E-03	2.080E-01	25	B003	2 2 2 2 2	
1.432E-03	1.520E-01	25	B060	2 0 1 1 1	
2.000E-03	2.123E-01	25	B153	2 1 1 1 2	
1.640E-03	1.741E-01	25	K001	1 0 2 1 2	
1.319E-03	1.400E-01	25	K072	1 0 1 1 1	
1.760E-03	1.869E-01	25	M342	1 0 1 1 2	
1.811E-03	1.923E-01	25	O312	2 2 0 2 2	
1.667E-03	1.770E-01	25	P003	2 2 2 2 2	
1.234E-03	1.310E-01	25	P051	2 1 1 2 2	
1.705E-03	1.810E-01	25	S203	1 1 2 1 2	
1.518E-03	1.612E-01	25	S358	2 1 2 2 2	
1.370E-03	1.455E-01	25	S359	2 1 2 2 2	
1.760E-03	1.869E-01	25	W300	2 2 2 2 2	
1.959E-03	2.080E-01	25.0	G035	1 0 0 0 2	
1.753E-03	1.861E-01	25.8	O312	2 2 0 2 2	
1.705E-03	1.810E-01	26.74	F418	0 0 0 0 0	
4.653E-03	4.940E-01	27	F185	1 0 0 0 2	
1.677E-03	1.780E-01	28	B348	2 1 2 2 2	
1.747E-03	1.855E-01	28	O312	2 2 0 2 2	
5.604E-03	5.950E-01	29	F185	1 0 0 0 2	
1.600E-03	1.698E-01	29.99	C350	0 0 0 0 0	
1.391E-03	1.477E-01	30	M311	1 1 2 2 2	
1.777E-03	1.887E-01	30	O312	2 2 0 2 2	
6.103E-03	6.480E-01	31	F185	1 0 0 0 2	
6.395E-03	6.790E-01	32	F185	1 0 0 0 2	
7.017E-03	7.450E-01	34	F185	1 0 0 0 2	
7.319E-03	7.770E-01	35	F185	1 0 0 0 2	
1.818E-03	1.930E-01	35	O312	2 2 0 2 2	
1.827E-03	1.940E-01	35	S203	1 1 2 1 2	

(*continued*)

1494. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.865E-03	8.350E-01	36	F185	1 0 0 0 2	
1.805E-03	1.917E-01	36.55	F418	0 0 0 0 0	
8.637E-03	9.170E-01	38	F185	1 0 0 0 2	
1.622E-03	1.722E-01	39.99	C350	0 0 0 0 0	
1.928E-03	2.047E-01	40	O312	2 2 0 2 2	
9.466E-03	1.005E+00	41	F185	1 0 0 0 2	
1.991E-03	2.114E-01	45	O312	2 2 0 2 2	
2.025E-03	2.150E-01	45	S203	1 1 2 1 2	
1.994E-03	2.117E-01	46.49	F418	0 0 0 0 0	
1.154E-02	1.225E+00	47	F185	1 0 0 0 2	
1.224E-02	1.300E+00	49	F185	1 0 0 0 2	
1.861E-03	1.976E-01	49.99	C350	0 0 0 0 0	
2.216E-03	2.353E-01	56.73	F418	0 0 0 0 0	
2.261E-03	2.400E-01	59.99	C350	0 0 0 0 0	
2.560E-03	2.718E-01	66.64	F418	0 0 0 0 0	
2.738E-03	2.907E-01	69.99	C350	0 0 0 0 0	
3.327E-03	3.532E-01	79.99	C350	0 0 0 0 0	
3.860E-03	4.098E-01	89.99	C350	0 0 0 0 0	
4.742E-03	5.035E-01	99.99	C350	0 0 0 0 0	
4.829E-03	5.127E-01	115.0	G035	1 0 0 0 2	
1.120E-02	1.189E+00	140.5	G035	1 0 0 0 2	
3.332E-02	3.537E+00	170.5	G035	1 0 0 0 2	
6.185E-02	6.567E+00	210.0	G035	1 0 0 0 2	
1.052E-01	1.116E+01	233.5	G035	1 0 0 0 2	
1.432E-03	1.520E-01	ns	H123	0 0 0 0 0	
6.300E-02	6.689E+00	ns	H307	0 0 0 0 0	
1.432E-03	1.520E-01	ns	M344	0 0 0 0 2	

1495. C_8H_{10}

m-Xylene
1,3-Xylene

RN: 108-38-3 **MP** (°C)**:** –47.4
MW: 106.17 **BP** (°C)**:** 139.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.846E-03	1.960E-01	0	P003	2 2 2 2 2	
1.463E-03	1.554E-01	20	M337	2 1 2 2 2	
1.629E-03	1.730E-01	25	A001	1 2 2 2 2	
1.846E-03	1.960E-01	25	B003	2 2 2 2 2	
1.262E-03	1.340E-01	25	K119	1 0 0 0 2	
1.510E-03	1.603E-01	25	M342	1 0 1 1 2	
1.526E-03	1.620E-01	25	P003	2 2 2 2 2	
1.262E-03	1.340E-01	25	P051	2 1 1 2 2	
1.375E-03	1.460E-01	25	S005	2 2 2 2 2	
1.375E-03	1.460E-01	25	S191	1 2 2 2 2	
1.375E-03	1.460E-01	25	S358	2 1 2 2 2	
1.330E-03	1.412E-01	25	S359	2 1 2 2 2	

(*continued*)

1495. C_8H_{10} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-03	1.603E-01	25	W300	2 2 2 2 2	
1.262E-03	1.340E-01	25.00	P007	2 1 2 2 2	
1.940E-03	2.059E-01	25.04	V013	2 2 2 2 2	
3.277E-03	3.479E-01	67.7	P005	1 1 2 1 2	
6.257E-03	6.643E-01	107.3	P005	1 1 2 1 2	
9.707E-03	1.031E+00	124.2	P005	1 1 2 1 2	
2.363E-02	2.509E+00	164.2	P005	1 1 2 1 2	
4.327E-02	4.594E+00	186.4	P005	1 1 2 1 2	
4.293E-02	4.557E+00	189.9	P005	1 1 2 1 2	
2.675E-01	2.840E+01	266.6	P005	1 1 2 1 2	
2.698E-01	2.865E+01	270.6	P005	1 1 2 1 2	

1496. C_8H_{10}

o-Xylene
1,2-Dimethylbenzene
1,2-Xylene

RN: 95-47-6 **MP** (°C)**:** –25
MW: 106.17 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.337E-03	1.420E-01	0	P003	2 2 2 2 2	
2.000E-03	2.123E-01	10	B149	2 1 1 2 2	
2.260E-03	2.399E-01	20	B149	2 1 1 2 2	
1.605E-03	1.704E-01	20	M337	2 1 2 2 2	
1.921E-03	2.040E-01	25	A001	1 2 2 2 2	
1.648E-03	1.750E-01	25	B060	2 0 1 1 1	
1.573E-03	1.670E-01	25	K119	1 0 0 0 2	
1.648E-03	1.750E-01	25	M001	2 1 2 2 2	
1.648E-03	1.750E-01	25	M002	2 1 2 2 2	
1.648E-03	1.750E-01	25	M040	1 0 0 1 2	
1.648E-03	1.750E-01	25	M130	1 0 0 0 2	
2.080E-03	2.208E-01	25	M342	1 0 1 1 2	
2.006E-03	2.130E-01	25	P003	2 2 2 2 2	
1.573E-03	1.670E-01	25	P051	2 1 1 2 2	
1.606E-03	1.705E-01	25	S005	2 2 2 2 2	
1.606E-03	1.705E-01	25	S191	1 2 2 2 2	
1.606E-03	1.705E-01	25	S358	2 1 2 2 2	
1.680E-03	1.784E-01	25	S359	2 1 2 2 2	
2.080E-03	2.208E-01	25	W300	2 2 2 2 2	
1.573E-03	1.670E-01	25.00	P007	2 1 2 2 2	
1.272E-03	1.350E-01	ns	B150	0 0 2 2 2	
1.648E-03	1.750E-01	ns	M344	0 0 0 0 2	

1497. C_8H_{10}
p-Xylene
1,4-Dimethylbenzene
1,4-Xylene
RN: 106-42-3 **MP** (°C)**:** 13
MW: 106.17 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.545E-03	1.640E-01	0	P003	2 2 2 2 2	
1.780E-03	1.890E-01	10	B149	2 1 1 2 2	
1.800E-03	1.911E-01	20	B149	2 1 1 2 2	
1.552E-03	1.648E-01	20	M337	2 1 2 2 2	
1.884E-03	2.000E-01	25	A001	1 2 2 2 2	
1.865E-03	1.980E-01	25	B003	2 2 2 2 2	
1.224E-03	1.300E-01	25	K072	1 0 1 1 1	
1.479E-03	1.570E-01	25	K119	1 0 0 0 2	
1.789E-03	1.900E-01	25	L319	1 0 2 1 1	
1.224E-03	1.300E-01	25	M087	1 1 2 1 1	
2.020E-03	2.145E-01	25	M342	1 0 1 1 2	
1.743E-03	1.850E-01	25	P003	2 2 2 2 2	
1.479E-03	1.570E-01	25	P051	2 1 1 2 2	
1.469E-03	1.560E-01	25	S005	2 2 2 2 2	
1.469E-03	1.560E-01	25	S191	1 2 2 2 2	
1.469E-03	1.560E-01	25	S358	2 1 2 2 2	
1.510E-03	1.603E-01	25	S359	2 1 2 2 2	
2.020E-03	2.145E-01	25	W300	2 2 2 2 2	
1.479E-03	1.570E-01	25.00	P007	2 1 2 2 2	
1.589E-03	1.687E-01	29.99	C350	0 0 0 0 0	
1.766E-03	1.875E-01	39.99	C350	0 0 0 0 0	
2.410E-03	2.559E-01	43.0	P005	1 1 2 1 2	
1.911E-03	2.029E-01	49.99	C350	0 0 0 0 0	
2.832E-03	3.007E-01	56.4	P005	1 1 2 1 2	
2.244E-03	2.382E-01	59.99	C350	0 0 0 0 0	
3.199E-03	3.396E-01	65.0	P005	1 1 2 1 2	
2.683E-03	2.848E-01	69.99	C350	0 0 0 0 0	
3.643E-03	3.868E-01	75.3	P005	1 1 2 1 2	
3.171E-03	3.367E-01	79.99	C350	0 0 0 0 0	
4.326E-03	4.593E-01	87.2	P005	1 1 2 1 2	
3.721E-03	3.950E-01	89.99	C350	0 0 0 0 0	
4.853E-03	5.152E-01	99.99	C350	0 0 0 0 0	
2.363E-02	2.509E+00	162.5	P005	1 1 2 1 2	
4.251E-02	4.513E+00	188.1	P005	1 1 2 1 2	
1.614E-01	1.713E+01	243.2	P005	1 1 2 1 2	
4.053E-01	4.303E+01	282.5	P005	1 1 2 1 2	
4.011E-01	4.258E+01	294.9	P005	1 1 2 1 2	
1.743E-03	1.850E-01	ns	H123	0 0 0 0 0	

1498. C_8H_{10}

Xylene
Dimethylbenzene
Xylol

RN: 1330-20-7 **MP** (°C)**:**
MW: 106.17 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-03	8.992E-01	20	C121	1 0 0 0 0	unit assumed, *sic*
1.000E-03	1.062E-01	25	H332	2 2 2 2 0	
<9.41E-03	<9.99E-01	25.50	O005	2 0 2 2 0	
9.419E-03	1.000E+00	150	J023	1 1 2 2 0	
3.297E-02	3.500E+00	200	J023	1 1 2 2 1	
1.036E-01	1.100E+01	250	J023	1 1 2 2 1	

1499. $C_8H_{10}NO_5PS$

Methyl parathion
Parathion-methyl
Methylparathion

RN: 298-00-0 **MP** (°C)**:** 36
MW: 263.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.282E-05	2.180E-02	10	B324	0 0 0 0 0	
8.283E-05	2.180E-02	10	B324	0 0 0 0 0	
1.432E-04	3.770E-02	19.50	B169	2 2 1 1 2	
1.444E-04	3.801E-02	20	B324	0 0 0 0 0	
1.444E-04	3.800E-02	20	B324	0 0 0 0 0	
9.498E-05	2.500E-02	20	M040	1 0 0 1 1	
2.090E-04	5.500E-02	25	M061	1 0 0 0 1	
2.185E-04	5.750E-02	25	M161	1 0 0 0 0	
2.089E-04	5.500E-02	25	Z409	0 0 0 0 0	EFG
2.223E-04	5.851E-02	30	B324	0 0 0 0 0	
2.222E-04	5.850E-02	30	B324	0 0 0 0 0	
1.900E-04	5.000E-02	ns	C117	0 0 0 0 0	
1.445E-04	3.805E-02	ns	R427	0 0 0 0 0	
1.432E-04	3.770E-02	ns	V414	0 0 0 0 0	

1500. $C_8H_{10}N_2O$

p-Phenylenediaminemono-*N*-acetate
p-Phenylendiamin-mono-*N*-acetat

RN: 589-29-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	6.200E+01	57	F300	1 0 0 0 1	

1501. $C_8H_{10}N_2O$
m-Aminoacetanilide
3-Aminoacetanilide
RN: 102-28-3 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.526E-01	8.299E+01	48.7	S115	1 2 1 1 2	
1.021E+00	1.534E+02	82.9	S115	1 2 1 1 2	

1502. $C_8H_{10}N_2O$
o-Aminoacetanilide
2-Aminoacetanilide
RN: 34801-09-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.189E-01	3.288E+01	7.2	S115	1 2 1 1 2	
7.161E-01	1.075E+02	22.0	S115	1 2 1 1 2	
1.215E+00	1.825E+02	33.5	S115	1 2 1 1 2	
1.612E+00	2.421E+02	42.1	S115	1 2 1 1 2	
1.958E+00	2.940E+02	50.4	S115	1 2 1 1 2	
2.270E+00	3.409E+02	59.1	S115	1 2 1 1 2	
2.601E+00	3.906E+02	69.9	S115	1 2 1 1 2	
2.781E+00	4.177E+02	78.2	S115	1 2 1 1 2	
2.943E+00	4.420E+02	88.1	S115	1 2 1 1 2	
3.075E+00	4.618E+02	99.0	S115	1 2 1 1 2	
3.213E+00	4.825E+02	115.4	S115	1 2 1 1 2	

1503. $C_8H_{10}N_2O$
1-(2-Tolyl)urea
o-Tolylurea
RN: 614-77-7 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-02	2.504E+00	45	W044	1 0 1 0 2	

1504. $C_8H_{10}N_2O$
1-Methyl-3-phenylurea
Desfenuron
N-Phenyl-*N′*-methylurea
Desphenuron
N-Methyl-*N′*-phenylurea
IPO 4328
RN: 1007-36-9 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E+00	7.400E+02	45	W044	1 0 1 0 2	

1505. $C_8H_{10}N_2O$
1-(4-Tolyl)urea
p-Tolylurea
RN: 622-51-5 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.044E-02	3.070E+00	45	W044	1 0 1 0 2	

1506. $C_8H_{10}N_2O$
p-Aminoacetanilide
4-Aminoacetanilide
RN: 122-80-5 **MP** (°C)**:** 164.5
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.061E-01	1.593E+01	25	D044	0 0 0 0 0	
4.064E-01	6.103E+01	56.8	S115	1 2 1 1 2	
1.046E+00	1.570E+02	86.3	S115	1 2 1 1 2	
1.441E+00	2.165E+02	92.1	S115	1 2 1 1 2	
1.699E+00	2.552E+02	93.7	S115	1 2 1 1 2	
1.996E+00	2.998E+02	96.5	S115	1 2 1 1 2	
2.193E+00	3.293E+02	98.6	S115	1 2 1 1 2	

1507. $C_8H_{10}N_2O$
Methylbenzylnitrosamine
N-Nitroso(methyl)benzylamine
N-Nitroso-*N*-methylbenzylamine
N-Nitroso(benzyl)methylamine
N-Nitroso-*N*-methylbenzenemethanamine
RN: 937-40-6 **MP** (°C)**:**
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	4.505E+00	24	D083	2 0 0 0 1	

1508. $C_8H_{10}N_2O$
Benzylurea
Benzyl-harnstoff
RN: 538-32-9 **MP** (°C)**:** 147
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-01	1.700E+01	45	F300	1 0 0 0 2	
1.139E-01	1.710E+01	45	W044	1 0 1 0 2	

1509. $C_8H_{10}N_2O_3$
5-Methyl-5-allylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(2-propenyl)
5-Methyl-5-allylbarbiturate
RN: 143585-01-7 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-02	1.261E+01	25	P350	0 0 0 0 0	intrinsic

1510. $C_8H_{10}N_2O_3$
5,5-Tetramethylenebarbituric acid
7,9-Diazaspiro[4.5]decane-6,8,10-trione
Spirocyclopentabarbituric acid
Cyclopentane-spirobarbiturate
RN: 56209-30-4 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.476E-03	8.154E-01	25	P350	0 0 0 0 0	intrinsic

1511. $C_8H_{10}N_2O_3S$
*N*1-Acetylsulfanilamide
Sulfacetamide
Acetyl sulfacetamide
RN: 144-80-9 **MP** (°C)**:** 183
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.881E-02	1.260E+01	20	F073	1 2 2 2 2	
3.871E-02	8.293E+00	25	M440	0 0 0 0 0	
5.834E-03	1.250E+00	37	B046	1 0 2 2 2	pH 4.5
5.834E-02	1.250E+01	37	B046	1 0 2 2 2	pH 5
6.908E-02	1.480E+01	37	D084	1 0 1 0 2	
5.601E-02	1.200E+01	37	K086	1 0 0 0 2	
5.134E-02	1.100E+01	37	L091	1 0 0 0 2	pH 5.5
2.327E-02	4.985E+00	ns	L044	0 0 0 0 2	
3.090E-02	6.621E+00	ns	R427	0 0 0 0 0	

1512. $C_8H_{10}N_2O_3S$
*N*4-Acetylsulfanilamide
*N*4-Acetylsulphanilamide
RN: 121-61-9 **MP** (°C)**:** 216
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.474E-02	5.300E+00	37	L091	1 0 0 0 2	pH 5.5
2.479E-02	5.312E+00	37.50	M142	1 0 0 0 2	

1513. $C_8H_{10}N_2O_3S$
Tosylurea
Tosyluree
RN: 1694-06-0 **MP** (°C)**:**
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.631E-03	7.779E-01	37	A028	1 0 2 1 2	intrinsic

1514. $C_8H_{10}N_2O_4S$

Asulam

Methyl *N*-(4-aminobenzenesulphonyl)carbamate

RN: 3337-71-1 **MP** (°C)**:** 144

MW: 230.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-02	4.975E+00	ns	M061	0 0 0 0 0	
2.188E-02	5.037E+00	ns	R427	0 0 0 0 0	
2.172E-02	5.000E+00	rt	M161	0 0 0 0 0	

1515. $C_8H_{10}N_4O_2$

Caffeine

Coffein

RN: 58-08-2 **MP** (°C)**:** 238

MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-02	7.548E+00	0	H023	1 0 2 1 2	
3.800E-02	7.379E+00	1	M116	2 1 1 1 1	
3.757E-02	7.296E+00	2	C074	1 0 0 1 2	
4.786E+00	9.294E+02	5	B429	1 0 1 2 2	
4.859E+00	9.436E+02	15	B429	1 0 1 2 2	
6.603E-02	1.282E+01	15	H023	1 0 2 1 2	
5.800E-02	1.126E+01	15	O017	1 0 1 1 1	
5.770E-02	1.121E+01	15	O018	1 2 1 1 2	
5.770E-02	1.121E+01	15	O019	1 0 0 1 2	
6.859E-02	1.332E+01	16	A072	1 0 1 0 2	
7.415E-02	1.440E+01	20	F300	1 0 0 0 2	
6.779E-02	1.316E+01	20	J009	2 0 2 2 2	
1.242E-01	2.411E+01	25	A068	2 0 0 0 2	
4.931E+00	9.575E+02	25	B429	1 0 1 2 2	
1.066E-01	2.071E+01	25	E016	1 1 1 1 2	
1.081E-01	2.100E+01	25	F300	1 0 0 0 1	
1.080E-01	2.097E+01	25	L329	2 2 1 2 2	
1.110E-01	2.156E+01	25	M116	2 1 1 1 2	
1.244E-01	2.415E+01	25	M158	2 0 2 2 2	
1.000E-01	1.942E+01	25	O017	1 0 1 1 2	
1.002E-01	1.946E+01	25	O018	1 2 1 1 2	
1.098E-02	2.132E+00	25	O019	1 0 0 1 2	
1.272E-01	2.470E+01	25	O302	1 0 0 1 0	
1.107E-01	2.150E+01	25	P010	1 0 1 1 2	
1.123E-01	2.180E+01	25	P011	0 0 0 0 0	
1.195E-01	2.320E+01	25	P018	1 0 2 2 2	
1.081E-01	2.100E+01	25	P020	2 0 1 1 1	
1.330E-01	2.583E+01	30	B042	1 2 1 1 2	
1.330E-01	2.583E+01	30	G021	1 0 0 0 2	
1.330E-01	2.583E+01	30	H020	1 0 0 0 2	
1.333E-01	2.589E+01	30	H023	1 0 2 1 2	

(*continued*)

1515. $C_8H_{10}N_4O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	2.583E+01	30.60	M116	2 1 1 1 2	
4.999E+00	9.707E+02	35	B429	1 0 1 2 2	
1.670E-01	3.243E+01	35	O017	1 0 1 1 2	
1.909E-01	3.707E+01	37	C074	1 0 0 1 2	
1.930E-01	3.748E+01	37	M116	2 1 1 1 2	
5.041E+00	9.789E+02	40	B429	1 0 1 2 2	
2.266E-01	4.400E+01	40	F300	1 0 0 0 1	
5.211E-01	1.012E+02	57	C074	1 0 0 1 2	
1.408E+00	2.735E+02	83	C065	1 0 0 1 2	
1.407E+00	2.733E+02	85	C074	1 0 0 1 2	
1.739E+00	3.377E+02	87	C065	1 0 0 1 2	
2.343E+00	4.550E+02	90	C074	1 0 0 1 2	
1.287E-01	2.500E+01	ns	D035	0 0 0 0 2	
1.104E-01	2.143E+01	rt	D021	0 0 1 1 2	
1.596E-04	3.100E-02	rt	N015	0 0 2 2 1	*sic*
4.892E-02	9.500E+00	rt	R431	0 0 0 0 0	Average

1516. $C_8H_{10}N_4O_2.H_2O$

Caffeine (monohydrate)

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-, monohydrate

RN: 5743-12-4 **MP** (°C)**:** 178

MW: 212.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-01	2.146E+01	25	D004	0 0 0 0 0	

1517. $C_8H_{10}N_4O_3$

1,3,7-Trimethyluric acid

8-Oxy-caffeine

RN: 5415-44-1 **MP** (°C)**:** 374

MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	2.400E-02	rt	N015	0 0 2 2 1	

1518. $C_8H_{10}O$
4-Ethylphenol
p-Ethylphenol
RN: 123-07-9 **MP** (°C)**:** 43.5
MW: 122.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.854E-02	5.931E+00	20	R087	0 0 0 0 0	0.15M NaCl
2.332E-02	2.849E+00	25	L022	1 0 0 0 0	
4.011E-02	4.900E+00	25	M127	1 0 0 0 1	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
4.467E-02	5.457E+00	ns	R427	0 0 0 0 0	

1519. $C_8H_{10}O$
2,3-Xylenol
2,3-Dimethylphenol
RN: 526-75-0 **MP** (°C)**:** 75
MW: 122.17 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.740E-02	4.569E+00	25	A021	1 2 1 1 2	

1520. $C_8H_{10}O$
Phenylethylalcohol
Phenyl ethyl alcohol
RN: 60-12-8 **MP** (°C)**:**
MW: 122.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-01	1.796E+01	20	S006	1 0 0 0 2	
1.720E-01	2.101E+01	25	D407	1 0 2 2 2	
1.432E-01	1.749E+01	25	H044	1 0 2 1 2	
1.455E-01	1.778E+01	30	H044	1 0 2 1 2	
1.487E-01	1.816E+01	35	H044	1 0 2 1 2	
1.518E-01	1.855E+01	40	H044	1 0 2 1 2	
1.542E-01	1.884E+01	45	H044	1 0 2 1 2	
1.562E-01	1.908E+01	50	H044	1 0 2 1 2	
1.597E-01	1.951E+01	55	H044	1 0 2 1 2	

1521. $C_8H_{10}O$
Phloral
RN: **MP** (°C)**:**
MW: 122.17 **BP** (°C)**:** 204.52

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-02	4.975E+00	25	L022	1 0 0 0 0	

1522. $C_8H_{10}O$
2,6-Xylenol
1,3,2-Xylenol
2,6-Dimethylphenol
Vic-*m*-xylenol
RN: 576-26-1 **MP** (°C)**:** 49
MW: 122.17 **BP** (°C)**:** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-02	4.392E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.950E-02	6.047E+00	25	A021	1 2 1 1 2	
5.100E-02	6.231E+00	25	B316	0 0 0 0 0	

1523. $C_8H_{10}O$
2,4-Xylenol
2,4-Dimethylphenol
m-Xylenol
2,4-Dimethyl-phenol-
Phenol, 2,4-dimethyl-
1-Hydroxy-2,4-dimethylbenzene
RN: 105-67-9 **MP** (°C)**:** 26
MW: 122.17 **BP** (°C)**:** 211.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-02	5.375E+00	20	K132	1 0 1 1 1	
4.300E-02	5.253E+00	20	K309	1 0 0 1 1	
5.271E-02	6.440E+00	20	R087	0 0 0 0 0	0.15M NaCl
5.100E-02	6.231E+00	25	A021	1 2 1 1 2	
6.440E-02	7.868E+00	25	B173	2 0 2 2 2	
7.200E-02	8.796E+00	25	B316	0 0 0 0 0	
6.499E-02	7.940E+00	25	M127	1 0 0 0 2	
2.190E-01	2.675E+01	80	K309	1 0 0 1 2	

1524. $C_8H_{10}O$
α-Methyl-benzenemethanol
α-Methylbenzyl alcohol
1-Phenylethan-1-*o*
Methylphenylcarbinol
β-Hydroxyethylbenzene
(*S*)-1-Phenylethyl alcohol
RN: 98-85-1 **MP** (°C)**:** 20
MW: 122.17 **BP** (°C)**:** 401 at 0 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E+00	8.427E+02	14.57	L441	0 0 0 0 0	
6.860E+00	8.380E+02	19.84	L441	0 0 0 0 0	

(*continued*)

1524. $C_8H_{10}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.056E-01	6.177E+01	92.71	L441	0 0 0 0 0	
6.491E+00	7.930E+02	94.89	L441	0 0 0 0 0	
6.445E+00	7.874E+02	105.95	L441	0 0 0 0 0	
6.196E+00	7.569E+02	127.92	L441	0 0 0 0 0	

1525. $C_8H_{10}O$

Phenetole
Ethoxybenzene

RN: 103-73-1 **MP** (°C)**:** –30
MW: 122.17 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	5.498E-01	25	M327	1 0 0 1 2	
4.657E-03	5.690E-01	25.04	V013	2 2 2 2 2	

1526. $C_8H_{10}O$

2,5-Xylenol
2,5-Dimethylphenol
p-Xylenol
2,5-Dimethyl-phenol-
Phenol, 2,5-dimethyl-

RN: 95-87-4 **MP** (°C)**:** 75
MW: 122.17 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	3.543E+00	25	A021	1 2 1 1 2	
2.600E-02	3.176E+00	25	B316	0 0 0 0 0	

1527. $C_8H_{10}O$

4-Methylbenzyl alcohol
4-Methyl-benzylalkohol

RN: 589-18-4 **MP** (°C)**:** 60
MW: 122.17 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-02	8.430E+00	20	B407	1 0 1 2 2	

1528. $C_8H_{10}O$
3,4-Xylenol
3,4-Dimethylphenol
As-*o*-xylenol
RN: 95-65-8 **MP** (°C)**:** 62.5
MW: 122.17 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	3.787E+00	20	K132	1 0 1 1 1	
3.900E-02	4.765E+00	25	A021	1 2 1 1 2	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
2.530E-02	3.091E+00	37	E028	1 0 1 1 2	

1529. $C_8H_{10}O$
3,5-Xylenol
3,5-Dimethylphenol
RN: 108-68-9 **MP** (°C)**:** 64
MW: 122.17 **BP** (°C)**:** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-02	4.032E+00	20	K132	1 0 1 1 1	
2.961E-02	3.618E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.000E-02	4.887E+00	25	A021	1 2 1 1 2	
4.000E-02	4.887E+00	25	B316	0 0 0 0 0	
3.981E-02	4.864E+00	ns	R427	0 0 0 0 0	

1530. $C_8H_{10}O_2$
o-Ethoxyphenol
2-Ethoxyphenol
RN: 94-71-3 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-02	8.414E+00	24.99	B353	0 0 0 0 0	

1531. $C_8H_{10}O_2$
Veratrole
o-Dimethoxybenzene
RN: 91-16-7 **MP** (°C)**:** 15
MW: 138.17 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.842E-02	6.690E+00	25	L348	1 2 2 1 2	

1532. $C_8H_{10}O_2$
1,3-Dimethoxybenzene
m-Dimethoxybenzene
Dimethylresorcinol
RN: 151-10-0 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:** 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.800E-03	1.216E+00	25	M327	1 0 0 1 2	

1533. $C_8H_{10}O_2$
2-Phenoxyethanol
Phenoxyethyl alcohol
Ethylene glycol phenyl ether
Arosol
1-Hydroxy-2-phenoxyethane
Phenoxethol
RN: 122-99-6 **MP** (°C)**:** 12
MW: 138.17 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.882E-01	2.601E+01	20	M062	1 0 0 0 2	
2.610E-01	3.606E+01	37	E028	1 0 1 1 2	

1534. $C_8H_{10}O_2$
3-Ethoxyphenol
m-Ethoxy phenol
Resorcinol monoethyl ether
RN: 621-34-1 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.382E+01	25	B314	0 0 0 0 0	
1.003E-01	1.386E+01	30	B315	0 0 0 0 0	

1535. $C_8H_{10}O_2$
p-Ethoxyphenol
Hydroquinone monoethyl ether
RN: 622-62-8 **MP** (°C)**:** 64.5–67.5
MW: 138.17 **BP** (°C)**:** 131 at 9 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.097E-02	7.043E+00	20	R087	0 0 0 0 0	0.15M NaCl

1536. $C_8H_{10}O_2$
p-Dimethoxybenzene
4-Dimethoxybenzene
RN: 150-78-7 **MP** (°C)**:**
MW: 138.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-05	7.641E-03	25	C316	0 0 0 0 0	0.1M NaCl

1537. $C_8H_{10}O_3$
1,3-Dimethyl ether pyrogallol
Pyrogallol-1,3-dimethylaether
2,6-Dimethoxyphenol
RN: 91-10-1 **MP** (°C)**:** 56
MW: 154.17 **BP** (°C)**:** 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.116E-01	1.720E+01	13	F300	1 0 0 0 2	

1538. $C_8H_{10}O_3S$
Benzene sulfonic acid ethyl ester
Ethyl benzenesulfonate
Ethyl phenylsulfonate
RN: 515-46-8 **MP** (°C)**:**
MW: 186.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.390E-03	1.376E+00	25	K097	2 0 2 2 2	

1539. $C_8H_{10}O_4$
Cyclohexene-1,4-dicarboxylic acid
Cyclohexen-(1)-dicarbonsaeure-(1,4)
RN: 2205-27-8 **MP** (°C)**:** 312
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-03	2.000E-01	20	F300	1 0 0 0 0	

1540. $C_8H_{10}O_4$
2-Cyclohexene-1,2-dicarboxylic acid
Cyclohexen-(2)-dicarbonsaeure-(1,2)
RN: 38765-78-5 **MP** (°C)**:**
MW: 170.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.113E-02	8.700E+00	10	F300	1 0 0 0 1	

1541. $C_8H_{10}O_5$
Endothall
Endothal
RN: 145-73-3 **MP** (°C)**:** 144
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.883E-01	9.091E+01	20	B200	1 0 0 0 2	
5.372E-01	1.000E+02	20	M161	1 0 0 0 2	
4.883E-01	9.091E+01	ns	B100	0 0 0 0 0	
4.883E-01	9.091E+01	ns	C307	0 0 0 0 1	

1542. $C_8H_{10}O_8$
meso-1,2,3,4-Butanetetracarboxylic acid
1,2,3,4-Butanetetracarboxylic acid
Butanetetracarboxylic acid
1,2,3,4,-Butane tetracarboxylic acid
RN: 1703-58-8 **MP** (°C)**:** 196
MW: 234.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.606E-01	1.547E+02	25	M370	1 2 2 1 2	

1543. $C_8H_{11}BrN_2O_2$
Isocil
Uracil, 5-bromo-3-isopropyl-6-methyl-
RN: 314-42-1 **MP** (°C)**:** 158–159
MW: 247.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.701E-03	2.150E+00	25	B185	0 0 0 0 0	

1544. $C_8H_{11}Cl_2NO$
N,N-Diallyldichloroacetamide
Dichlormid
N,N-Diallyl dichloroacetamide
2,2-Dichloro-*N,N*-di-2-propenylacetamide
R 25788
RN: 37764-25-3 **MP** (°C)**:** 5
MW: 208.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.403E-02	5.000E+00	20	M161	1 0 0 0 0	
2.399E-02	4.992E+00	ns	S460	0 0 0 0 0	

1545. $C_8H_{11}Cl_3O_6$
Chloralose
1,2-*O*-(2,2,2-Trichloroethylidene)-α-D-glucofuranose
Anhydroglucochloral
Alfamat
Aphosal
Murex
RN: 15879-93-3 **MP** (°C)**:** 187
MW: 309.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-02	4.440E+00	15	M161	1 0 0 0 2	

1546. $C_8H_{11}N$
Xylidine
N,N-Dimethylaniline
Dimethylaminobenzene
Benzenamine
Aminodimethylbenzene
RN: 121-69-7 **MP** (°C)**:** 2
MW: 121.18 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.120E-03	1.105E+00	25	C113	1 0 2 1 2	

1547. $C_8H_{11}NO$
Tyramine
Tyramin
4-Hydroxyphenylethylamine
4-(2-Aminoethyl)phenol
2-(*p*-Hydroxyphenyl)ethylamine
RN: 51-67-2 **MP** (°C)**:** 164.5
MW: 137.18 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.574E-02	1.039E+01	15	D041	1 0 0 0 2	
7.581E-02	1.040E+01	15	F300	1 0 0 0 2	

1548. $C_8H_{11}NO$
Phenylethanolamine
Phenyl ethanolamine
2-Anilinoethanol
β-Hydroxyethyl aniline
N-Phenylethanolamine
PEA
RN: 7568-93-6 **MP** (°C)**:** 56.5
MW: 137.18 **BP** (°C)**:** 286.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.192E-01	4.379E+01	20	M062	1 0 0 0 2	

1549. $C_8H_{11}N_2O_5PS$
Parathion-amino
Aminoparathion
RN: **MP** (°C)**:**
MW: 278.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.419E-03	3.948E-01	19.50	B169	2 2 1 1 2	

1550. $C_8H_{11}N_3O_3S$
Lamivudine
2(1H)-Pyrimidinone,4-amino-1-[2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-,(2R-*cis*)
Epivir
3′-Thia-2′,3′-dideoxcytidine
(–)NGPB-21
(–) 2′-Deoxy-3′-thiacytidine
RN: 134678-17-4 **MP** (°C)**:**
MW: 229.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-01	7.000E+01	ns	K444	0 0 0 0 0	
3.053E-01	7.000E+01	rt	B435	0 0 0 0 0	

1551. $C_8H_{11}N_5O_3$
Acyclovir
Acycloguanosine
9-(2-Hydroxyethoxymethyl)guanine
6H-Purin-6-one, 2-amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]-
Cargosil
Zovirax
RN: 59277-89-3 **MP** (°C)**:**
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.216E-03	1.400E+00	21	B419	1 1 2 2 1	int
7.150E-03	1.610E+00	22	K443	0 0 0 0 0	
7.244E-03	1.631E+00	22	K445	0 0 0 0 0	
5.380E-03	1.212E+00	22.5	B422	2 0 2 2 2	
2.240E+00	5.045E+02	25	B443	0 0 0 0 0	
8.070E-03	1.817E+00	25	Z407	0 0 0 0 0	
4.440E-02	1.000E+01	ns	K444	0 0 0 0 0	
6.166E-03	1.389E+00	ns	R427	0 0 0 0 0	

1552. C_8H_{12}
4-Vinylcyclohexene
4-Vinyl-1-cyclohexene
RN: 100-40-3 **MP** (°C)**:** –101
MW: 108.18 **BP** (°C)**:** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.622E-04	5.000E-02	25	M001	2 1 2 2 1	

1553. $C_8H_{12}ClNO$
Allidochlor
CDAA
N,N-Diallyl-2-chloroacetamide
Randox
2-Chloro-*N,N*-diallylacetamide
CP 6343
RN: 93-71-0 **MP** (°C)**:**
MW: 173.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.113E-01	1.932E+01	22	J008	1 0 0 0 2	
1.113E-01	1.932E+01	25	B185	0 0 0 0 0	
1.135E-01	1.970E+01	25	G319	0 0 0 0 0	
1.135E-01	1.970E+01	25	M161	1 0 0 0 2	
1.129E-01	1.961E+01	ns	B100	0 0 0 0 0	
1.130E-01	1.962E+01	ns	F184	0 0 0 0 2	
1.129E-01	1.961E+01	ns	M061	0 0 0 0 0	
3.162E-01	5.491E+01	ns	M163	0 0 0 0 0	EFG

1554. $C_8H_{12}N_2O_2S$

*N*1-Dimethylsulfanilamide
p-Amino-*N,N*-dimethylbenzenesulfonamide
[(4-Aminophenyl)sulfonyl]dimethylamine
p-(Dimethylsulfamoyl)aniline

RN: 1709-59-7 **MP** (°C)**:**
MW: 200.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	6.268E-01	37	K095	2 0 0 0 2	intrinsic

1555. $C_8H_{12}N_2O_2S$

5,5-Diethyl-2-thiobarbituric acid
4,6(1H,5H)-Pyrimidinedione, 5,5-diethyldihydro-2-thioxo
Barbituric acid, 5,5-diethyl-2-thio
Certodorm

RN: 77-32-7 **MP** (°C)**:**
MW: 200.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.810E-03	1.364E+00	25	P350	0 0 0 0 0	intrinsic

1556. $C_8H_{12}N_2O_3$

Barbital
5,5-Diethylbarbituric acid
Diethylmalonylurea

RN: 57-44-3 **MP** (°C)**:** 190
MW: 184.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.131E+00	0	M143	1 2 1 1 0	
1.900E-02	3.500E+00	0	M143	1 2 1 1 2	
2.562E-02	4.720E+00	10	N007	1 2 2 2 2	form I
1.900E-02	3.500E+00	10	N007	1 2 2 2 2	form III
3.100E-02	5.710E+00	14	I006	1 0 0 0 1	
3.187E-02	5.870E+00	15	H018	0 0 0 0 0	
3.500E-02	6.447E+00	19	I006	1 0 0 0 1	
4.522E-02	8.330E+00	20	D041	1 0 0 0 1	
3.637E-02	6.700E+00	20	F300	1 0 0 0 1	
3.415E-02	6.290E+00	20	J030	1 2 2 2 2	
2.839E-02	5.230E+00	20	N007	1 2 2 2 2	form III
3.409E-02	6.280E+00	20	N007	1 2 2 2 2	form I
3.806E-02	7.011E+00	20	S146	2 2 2 1 2	form I
3.752E-02	6.912E+00	20	S146	2 2 2 1 2	form II
3.881E-02	7.149E+00	25	A023	1 0 0 1 2	
3.963E-02	7.300E+00	25	B011	2 0 0 1 0	
3.971E-02	7.314E+00	25	B065	1 1 1 1 1	
3.746E-02	6.900E+00	25	B167	1 1 0 0 1	pH 5.7

(*continued*)

1556. $C_8H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-02	7.110E+00	25	G003	1 1 1 1 2	pH 4.7
2.800E-02	5.158E+00	25	M143	1 2 1 1 2	
4.050E-02	7.460E+00	25	M310	2 2 2 2 2	
4.018E-02	7.401E+00	25	P350	0 0 0 0 0	intrinsic
4.239E-02	7.809E+00	25	S146	2 2 2 1 2	form II
4.010E-03	7.386E-01	25	V033	2 0 1 1 2	
4.010E-02	7.386E+00	25.00	T303	1 0 0 0 2	
4.300E-02	7.920E+00	27	I006	1 0 0 0 1	
4.300E-02	7.920E+00	30	G014	1 1 1 1 0	EFG, 0.003N H_2SO_4
2.704E-02	4.980E+00	30	H005	1 0 1 2 2	average of 4
4.408E-02	8.119E+00	30	H018	0 0 0 0 0	
4.400E-02	8.105E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
4.260E-02	7.847E+00	30	K108	1 2 2 0 2	
4.425E-02	8.150E+00	30	N007	1 2 2 2 2	form I
4.207E-02	7.750E+00	30	N007	1 2 2 2 2	form III
4.720E-02	8.694E+00	30	S146	2 2 2 1 2	form I
4.618E-02	8.507E+00	30	S146	2 2 2 1 2	form II
5.162E-02	9.509E+00	35	S146	2 2 2 1 2	form I
5.184E-02	9.548E+00	35	S146	2 2 2 1 2	form II
5.150E-02	9.486E+00	35.00	T303	1 0 0 0 2	
4.843E-02	8.920E+00	36	A023	1 0 0 1 2	
5.152E-02	9.490E+00	37	J030	1 2 2 2 2	
5.300E-02	9.762E+00	37	K121	1 2 1 2 1	0.1N HCl
5.538E-02	1.020E+01	37	N007	1 2 2 2 2	form III
5.277E-02	9.720E+00	37	N007	1 2 2 2 2	form I
5.668E-02	1.044E+01	37	S146	2 2 2 1 2	form II
5.588E-02	1.029E+01	40	A023	1 0 0 1 1	
6.100E-01	1.124E+02	40	N008	1 0 1 1 2	*sic*
6.967E-02	1.283E+01	45	S146	2 2 2 1 2	form II
6.800E-02	1.253E+01	45.00	T303	1 0 0 0 2	
4.343E-01	8.000E+01	100	F300	1 0 0 0 1	
3.257E-02	6.000E+00	ns	T003	0 0 0 0 2	

1557. $C_8H_{12}O_2$

1-Epoxyethyl-3,4-epoxycyclohexane
Vinylcyclohexene dioxide

RN: 106-87-6 **MP** (°C)**:** <–55
MW: 140.18 **BP** (°C)**:** 227

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E+00	1.547E+02	20	I313	0 0 0 0 0	

1558. $C_8H_{12}O_4$
trans-Cyclohexane-1,2-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,2)
RN: 2305-32-0 **MP** (°C)**:**
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-02	2.000E+00	20	F300	1 0 0 0 0	

1559. $C_8H_{12}O_4$
cis-Cyclohexane-1,2-dicarboxylic acid
cis-Cyclohexan-dicarbonsaeure-(1,2)
RN: 610-09-3 **MP** (°C)**:** 193
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.16E-02	>2.00E+00	20	F300	1 0 0 0 0	

1560. $C_8H_{12}O_4$
trans-Cyclohexane-1,4-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,4)
RN: 619-82-9 **MP** (°C)**:**
MW: 172.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.646E-03	8.000E-01	17	F300	1 0 0 0 0	
7.550E-02	1.300E+01	100	F300	1 0 0 0 1	

1561. $C_8H_{13}BrN_2O_2$
α-Bromethylpropylaceturea
RN: **MP** (°C)**:**
MW: 249.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-03	4.098E-01	20	O021	1 0 0 0 0	

1562. $C_8H_{13}NO$
Diaalylacetamide
α,α-Diallylacetamide
2-(2-Propenyl)4-pentenamide
RN: 60730-94-1 **MP** (°C)**:**
MW: 139.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.750E+01	ns	H348	0 0 0 0 0	

1563. $C_8H_{13}N_2O_3PS$
Thionazin
O,O-Diethyl *O*-pyrazinyl thiophosphate
RN: 297-97-2 **MP** (°C)**:** –1.7
MW: 248.24 **BP** (°C)**:** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.140E+00	25	M061	1 0 0 0 2	
4.592E-03	1.140E+00	27	M161	1 0 0 0 2	

1564. C_8H_{14}
1-Octyne
Hexylacetylene
n-Hexylacetylene
RN: 629-05-0 **MP** (°C)**:** –80
MW: 110.20 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.178E-04	2.400E-02	25	M001	2 1 2 2 2	

1565. C_8H_{14}
2,2-Dimethyl-3-hexyne
1-Ethyl-2-tertbutylacetylene
RN: 4911-60-8 **MP** (°C)**:**
MW: 110.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	7.934E-02	25	H039	1 2 2 2 1	

1566. $C_8H_{14}ClNS_2$
Carbamic acid, diethyldithio-2chloroallyl ester
2-Chloroallyl diethyldithiocarbamate
CDEC
RN: 95-06-7 **MP** (°C)**:** <25
MW: 223.79 **BP** (°C)**:** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.469E-04	1.000E-01	25	B185	0 0 0 0 0	
4.111E-04	9.200E-02	25	B200	1 0 0 0 1	
4.469E-04	1.000E-01	25	F019	1 0 0 0 2	
4.111E-04	9.200E-02	25	G319	0 0 0 0 0	
4.111E-04	9.200E-02	25	M161	1 0 0 0 1	
4.468E-04	9.999E-02	ns	M061	0 0 0 0 0	approximate

1567. $C_8H_{14}ClN_5$
Atrazine
2-Chloro-4-ethylamino-6-isopropylamino-*s*-triazine
RN: 1912-24-9 **MP** (°C)**:** 172
MW: 215.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-04	2.200E-02	0	B185	0 0 0 0 0	
1.390E-04	2.998E-02	1	G091	1 0 1 2 2	pH 6.0
5.000E-04	1.078E-01	2	B193	1 2 0 0 0	
1.410E-04	3.041E-02	8	G091	1 0 1 2 2	pH 6.0
1.530E-04	3.300E-02	20	A314	0 0 0 0 0	
1.345E-04	2.900E-02	20	C048	2 2 2 2 1	
1.391E-04	3.000E-02	20	E048	1 2 1 1 1	
1.391E-04	3.000E-02	20	F311	1 2 2 2 1	
1.580E-04	3.408E-02	20	G091	1 0 1 2 2	pH 6.0
1.298E-04	2.800E-02	20	M161	1 0 0 0 1	
1.391E-04	3.000E-02	20	N333	0 0 0 0 0	
3.245E-04	7.000E-02	21	B192	0 0 0 0 1	
3.245E-04	7.000E-02	21	G099	2 0 0 1 0	
3.245E-04	7.000E-02	22	M061	1 0 0 0 1	
1.530E-04	3.300E-02	25	H024	2 2 2 2 2	
1.386E-04	2.990E-02	25	H073	2 1 1 2 2	
1.530E-04	3.300E-02	25	P434	0 0 0 0 0	
3.245E-04	7.000E-02	27	B185	0 0 0 0 0	
1.530E-04	3.300E-02	27	B200	1 0 0 0 1	
1.970E-04	4.249E-02	29	G091	1 0 1 2 2	pH 6.0
4.530E-04	9.771E-02	50	G001	1 0 0 1 2	
1.484E-03	3.200E-01	85	B185	0 0 0 0 0	
3.245E-04	7.000E-02	ns	C101	0 0 0 0 1	
3.245E-04	7.000E-02	ns	G041	0 0 0 0 1	
3.245E-04	7.000E-02	ns	H112	0 0 0 0 1	
1.530E-04	3.300E-02	ns	J033	0 0 0 0 0	
3.941E-04	8.500E-02	ns	M110	0 0 0 0 0	EFG
1.609E-04	3.470E-02	ns	V414	0 0 0 0 0	

1568. $C_8H_{14}N_2O_2$
cis-N,N,N′,N′-Tetramethylfumaramide
2-Butenediamide, *N,N,N′,N′*-tetramethyl-, (Z)-
RN: 35075-35-5 **MP** (°C)**:**
MW: 170.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E+00	2.945E+02	30	K019	1 0 0 0 2	

1569. $C_8H_{14}N_4OS$
Metribuzin
4-Amino-6-*tert*-butyl-3-(methylthio)-as-triazin-5(4H)-one
Bayer 6159H
Lexone
Sencor
Sencorex
RN: 21087-64-9 **MP** (°C)**:** 125.8
MW: 214.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	1.200E+00	20	M161	1 0 0 0 1	
5.693E-03	1.220E+00	22.5	G301	0 0 0 0 0	
4.662E-03	9.990E-01	ns	B100	0 0 0 0 0	
7.000E-03	1.500E+00	ns	M110	0 0 0 0 0	EFG

1570. $C_8H_{14}O$
Bicyclo[2.2.1]heptylcarbinol
2-Norcamphanemethanol
RN: 5240-72-2 **MP** (°C)**:**
MW: 126.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.916E-03	9.990E-01	ns	M061	0 0 0 0 0	

1571. $C_8H_{14}O_2$
2,4-Octadione
Valerylacetone
RN: 14090-87-0 **MP** (°C)**:**
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.925E+00	25	M078	2 0 1 0 2	

1572. $C_8H_{14}O_2$
Cyclohexanol acetate
Hexalin acetate
Cyclohexyl acetate
RN: 622-45-7 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.597E+00	20	D052	1 1 0 0 1	
2.033E-02	2.892E+00	23.50	O005	2 0 2 2 1	
2.138E-02	3.040E+00	ns	S460	0 0 0 0 0	

1573. $C_8H_{14}O_2$
6-Methyl-2,4-heptadione
2-Methyl-4,6-heptanedione
Isovalerylacetone
RN: 3002-23-1 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.490E-02	3.541E+00	25	M078	2 0 1 0 2	

1574. $C_8H_{14}O_2$
3-Propyl-2,4-pentadione
3-Acetyl-2-hexanone
RN: 1540-35-8 **MP** (°C)**:** <25
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	1.891E+01	25	M078	2 0 1 0 2	

1575. $C_8H_{14}O_2$
5,5-Dimethyl-2,4-hexadione
Pivaloylacetone
Pivaloylacetylmethane
RN: 7307-04-2 **MP** (°C)**:**
MW: 142.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-02	3.327E+00	25	M078	2 0 1 0 2	

1576. $C_8H_{14}O_2S_4$
Propyl dixanthogen
bis(1-Propyl) dixanthogen
Propyl xanthogen disulfide
Dipropyl dixanthogen
Dipropyl thioperoxydicarbonate
Dipropyl xanthogen disulfide
RN: 3750-28-5 **MP** (°C)**:**
MW: 270.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.057E-04	25	H102	1 2 1 2 1	

1577. $C_8H_{14}O_4$
Suberic acid
Korksaeure
RN: 505-48-6 **MP** (°C)**:** 142
MW: 174.20 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	8.000E-01	0	L041	1 0 0 1 0	
5.301E-03	9.234E-01	6.99	A340	0 0 0 0 0	
7.097E-03	1.236E+00	12.69	A340	0 0 0 0 0	
8.037E-03	1.400E+00	15	F300	1 0 0 0 1	
7.463E-03	1.300E+00	15	L041	1 0 0 1 1	
7.463E-03	1.300E+00	15	M051	1 0 0 0 1	
9.789E-03	1.705E+00	18.69	A340	0 0 0 0 0	
9.185E-03	1.600E+00	20	L041	1 0 0 1 1	
8.986E-03	1.565E+00	20	M171	1 0 0 0 0	
1.206E-01	2.100E+01	21	B040	1 0 1 1 2	*sic*
1.388E-02	2.417E+00	24.99	A340	0 0 0 0 0	
3.387E-02	5.900E+00	25	F300	1 0 0 0 1	
6.800E-02	1.185E+01	25	K040	1 0 2 1 2	*sic*
1.700E-02	2.961E+00	30	H021	1 0 1 1 0	EFG
1.890E-02	3.293E+00	32.49	A340	0 0 0 0 0	
2.045E-02	3.563E+00	34.49	A340	0 0 0 0 0	
2.583E-02	4.500E+00	35	L041	1 0 0 1 1	
2.326E-02	4.051E+00	39.99	A340	0 0 0 0 0	
2.682E-02	4.673E+00	44.49	A340	0 0 0 0 0	
5.626E-02	9.800E+00	50	L041	1 0 0 1 1	
3.198E-02	5.571E+00	50.19	A340	0 0 0 0 0	
3.534E-02	6.156E+00	52.69	A340	0 0 0 0 0	
5.551E-02	9.670E+00	61.49	A340	0 0 0 0 0	
6.422E-02	1.119E+01	63.99	A340	0 0 0 0 0	
1.274E-01	2.220E+01	65	L041	1 0 0 1 2	
8.182E-02	1.425E+01	70.09	A340	0 0 0 0 0	
1.156E-01	2.013E+01	76.49	A340	0 0 0 0 0	
1.386E-02	2.414E+00	rt	H431	0 0 0 0 0	

1578. $C_8H_{14}O_4$
Diethyl succinate
Butanedioic acid, diethyl ester
RN: 123-25-1 **MP** (°C)**:** –20
MW: 174.20 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.089E-02	1.896E+00	ns	F014	0 0 0 0 2	

1579. $C_8H_{14}O_4$
Butylene glycol diacetate
1,4-Diacetoxybutane
Tetramethylene acetate
RN: 628-67-1 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.005E-01	3.494E+01	26	O012	1 2 1 1 2	
1.602E-01	2.790E+01	50	O012	1 2 1 1 2	
2.048E-01	3.568E+01	75	O012	1 2 1 1 2	

1580. $C_8H_{14}O_4$
Tetramethyl succinic acid
Tetramethyl-bernsteinsaeure
RN: 630-51-3 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.755E-02	4.800E+00	13.5	F300	1 0 0 0 1	

1581. $C_8H_{14}O_4$
Isoamylmalonic acid
Acide isoamylmalonique
RN: 616-87-5 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E+00	3.850E+02	0	M051	1 0 0 0 2	
2.974E+00	5.180E+02	15	M051	1 0 0 0 2	
3.490E+00	6.080E+02	25	M051	1 0 0 0 2	
4.788E+00	8.340E+02	50	M051	1 0 0 0 2	

1582. $C_8H_{14}O_4$
Propyl α-acetoxypropionate
Hydracrylic acid, propyl ester, acetate
RN: 20473-73-8 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.683E-02	9.900E+00	25	R006	2 2 0 1 1	

1583. $C_8H_{14}O_4$
Ethylene glycol dipropionate
1,2-Ethanediol, dipropanoate
1,2-bis(Propionyloxy)ethane
RN: 123-80-8 **MP** (°C)**:**
MW: 174.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.480E-02	1.651E+01	25	F064	1 0 0 0 2	
9.170E-03	1.597E+00	ns	F014	0 0 0 0 2	

1584. $C_8H_{14}O_5$
Propanoic acid, 2-[(propoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 190.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	5.173E+00	25	R007	0 0 0 0 0	

1585. $C_8H_{15}ClN_5O$
Hydroxyatrazine
4-(Ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2(1H)-one
2-Hydroxy atrazine
RN: 2163-68-0 **MP** (°C)**:**
MW: 232.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.585E-02	2	B193	1 2 0 0 1	

1586. $C_8H_{15}NO$
Pelletierine
Pelletierin
RN: 2858-66-4 **MP** (°C)**:** <25
MW: 141.21 **BP** (°C)**:** 195

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-01	5.000E+01	20	F300	1 0 0 0 0	
3.372E-01	4.762E+01	25	D004	0 0 0 0 0	

1587. $C_8H_{15}NO$
Propylallylacetamide
2-Propyl-4-pentenamide
PAD
RN: 90204-40-3 **MP** (°C)**:**
MW: 141.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-02	9.500E+00	37	H347	0 0 0 0 0	

1588. $C_8H_{15}NO_2S$
4-Thiazolidinecarboxylic acid, 2-butyl-
RN: 90205-28-0 **MP** (°C)**:**
MW: 189.28 **BP** (°C)**:** 355.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.079E+01	21	B414	1 0 0 1 1	partial decomposition

1589. $C_8H_{15}NO_2S$
4-Thiazolidinecarboxylic acid, 2-(2-methylpropyl)-
4-Thiazolidine-4-carboxylic acid, 2-(2-isobutyl)-
RN: 215669-71-9 **MP** (°C)**:**
MW: 189.28 **BP** (°C)**:** 347.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	9.275E+00	21	B414	1 0 0 1 1	partial decomposition

1590. $C_8H_{15}N_3O_2$
Isocarbamid
N-(2-Methylpropyl)-2-oxo-1-imidazolidinecarboxamide
RN: 30979-48-7 **MP** (°C)**:** 95.5
MW: 185.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.018E-03	1.300E+00	20	M161	1 0 0 0 1	

1591. $C_8H_{15}N_3O_7$

Streptozotocin
Streptozocin
D-2-Deoxy-2-(3-methyl-3-nitrosoureido)glucopyranose
RN: 18883-66-4 **MP** (°C)**:** 115
MW: 265.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-02	5.066E+00	25	I307	0 0 0 0 0	

1592. $C_8H_{15}N_5O$

Simetone
2-Methoxy-4,6-bis(ethylamino)-*s*-triazine
s-Triazole, 2,4-bis(ethylamine)-6-methoxy-
RN: 673-04-1 **MP** (°C)**:** 118-120
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.622E-02	3.200E+00	21	B185	0 0 0 0 0	
1.622E-02	3.200E+00	21	B192	0 0 0 0 2	
1.622E-02	3.200E+00	21	G099	2 0 0 1 0	
3.550E-02	7.002E+00	50	G001	1 0 1 1 2	
1.622E-02	3.200E+00	ns	C101	0 0 0 0 1	

1593. $C_8H_{15}N_5O$

2-Methoxy-4-methylamino-6-isopropylamino-*s*-triazine
Noratone
RN: 3035-45-8 **MP** (°C)**:**
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.774E-02	3.500E+00	20	J033	0 0 0 0 0	
1.774E-02	3.500E+00	21	B192	0 0 0 0 2	

1594. $C_8H_{15}N_5S$

Desmetryne
N-Methyl-*N*′-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
Semeron
Methylamino-4-methylthio-6-isopropylamino-1,3,5-triazine
Topusyn
Methylthio-4-isopropylamino-6-methylamino-*s*-triazine
RN: 1014-69-3 **MP** (°C)**:**
MW: 213.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-03	6.000E-01	20	F311	1 2 2 2 1	
2.719E-03	5.800E-01	20	M161	1 0 0 0 2	
2.811E-03	5.996E-01	ns	B100	0 0 0 0 0	

(*continued*)

1594. $C_8H_{15}N_5S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	5.800E-01	ns	J033	0 0 0 0 0	
2.719E-03	5.800E-01	ns	M061	0 0 0 0 2	

1595. $C_8H_{15}N_5S$

Simetryne
N,N′-Diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
G-32911
bis(Ethylamino)-6-(methylthio)-*s*-triazine
Methylthio-4,6-bis(ethylamino)-*s*-triazine
Cymetrin

RN: 1014-70-6 **MP** (°C)**:** 82
MW: 213.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	1.003E+00	50	G001	1 0 1 1 1	
2.110E-03	4.500E-01	ns	C101	0 0 0 0 1	
2.110E-03	4.500E-01	ns	J033	0 0 0 0 0	
2.110E-03	4.500E-01	rt	M161	0 0 0 0 2	

1596. $C_8H_{15}N_7O_2S_3$

Famotidine
Amfamox
N′-(Aminosulfonyl)-3-(((2-(((diaminomethylene)amino)-4-thiazolyl)methyl)thio)propanimidamide
Pepcid
Pepcidine
Pepcid PM

RN: 76824-35-6 **MP** (°C)**:**
MW: 337.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.260E-06	1.100E-03	25	A408	2 0 1 2 0	
3.311E-03	1.117E+00	ns	R427	0 0 0 0 0	

1597. C_8H_{16}

Cyclooctane

RN: 292-64-8 **MP** (°C)**:** 10
MW: 112.22 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-03	1.817E-01	20	M337	2 1 2 2 2	*sic*
7.040E-05	7.900E-03	25	M001	2 1 2 2 1	
7.040E-05	7.900E-03	ns	H123	0 0 0 0 0	

1598. C_8H_{16}
Caprylene
1-Octene
RN: 111-66-0 **MP** (°C)**:** –102
MW: 112.22 **BP** (°C)**:** 121.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-05	3.600E-03	23	C332	0 0 0 0 0	
2.406E-05	2.700E-03	25	M001	2 1 2 2 1	
3.650E-05	4.096E-03	25	M342	1 0 1 1 2	

1599. C_8H_{16}
1,4-Dimethylcyclohexane
p-Dimethylcyclohexane
RN: 589-90-2 **MP** (°C)**:** –87
MW: 112.22 **BP** (°C)**:** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	K119	1 0 0 0 2	

1600. C_8H_{16}
cis-1,2-Dimethylcyclohexane
1-*cis*-2-Dimethylcyclohexane
RN: 2207-01-4 **MP** (°C)**:** –50
MW: 112.22 **BP** (°C)**:** 129

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.773E-05	7.600E-03	20	M337	2 1 2 2 1	
5.347E-05	6.000E-03	25	M001	2 1 2 2 1	

1601. C_8H_{16}
n-Propylcyclopentane
1-Propylcyclopentane
RN: 2040-96-2 **MP** (°C)**:** –117
MW: 112.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.818E-05	2.040E-03	25	K119	1 0 0 0 2	
1.818E-05	2.040E-03	25	P051	2 1 1 2 2	
1.818E-05	2.040E-03	25.00	P007	2 1 2 2 2	

1602. C_8H_{16}
trans-1,2-Dimethylcyclohexane
1,2-*trans*-Dimethylcyclohexane
RN: 6876-23-9 **MP** (°C)**:** –89
MW: 112.22 **BP** (°C)**:** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-05	5.200E-03	20	M337	2 1 2 2 1	
4.444E-05	4.987E-03	30.2	M447	0 0 0 0 0	
1.061E-04	1.191E-02	70.3	M447	0 0 0 0 0	
2.611E-04	2.930E-02	100.7	M447	0 0 0 0 0	
6.000E-04	6.733E-02	131.0	M447	0 0 0 0 0	
1.239E-03	1.390E-01	151.0	M447	0 0 0 0 0	
1.977E-03	2.219E-01	170.1	M447	0 0 0 0 0	

1603. C_8H_{16}
trans-1,4-Dimethylcyclohexane
1,4-Transdimethylcyclohexane
RN: 2207-04-7 **MP** (°C)**:** –37
MW: 112.22 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	P051	2 1 1 2 2	
3.422E-05	3.840E-03	25.00	P007	2 1 2 2 2	

1604. C_8H_{16}
1,2-Dimethylcyclohexane (*cis* + *trans*)
Cyclohexane, 1,2-dimethyl- (*cis*/*trans*)
1,2-Dimethylcyclohexane
RN: 583-57-3 **MP** (°C)**:**
MW: 112.22 **BP** (°C)**:** 124 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.056E-05	6.795E-03	30.0	M447	0 0 0 0 0	
1.200E-04	1.347E-02	70.0	M447	0 0 0 0 0	
2.422E-04	2.718E-02	100.2	M447	0 0 0 0 0	
5.483E-04	6.153E-02	130.5	M447	0 0 0 0 0	
1.089E-03	1.222E-01	150.5	M447	0 0 0 0 0	
2.422E-03	2.717E-01	170.5	M447	0 0 0 0 0	

1605. C_8H_{16}
1,1,3-Trimethylcyclopentane
Cyclopentane, 1,1,3-trimethyl-
RN: 4516-69-2 **MP** (°C)**:** –142.4
MW: 112.22 **BP** (°C)**:** 104.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.324E-05	3.730E-03	25	K119	1 0 0 0 2	
3.324E-05	3.730E-03	25	P051	2 1 1 2 2	
3.324E-05	3.730E-03	25.00	P007	2 1 2 2 2	

1606. C_8H_{16}
Ethyl cyclohexane
Cyclohexane, ethyl-
RN: 1678-91-7 **MP** (°C)**:**
MW: 112.22 **BP** (°C)**:** 131.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.614E-05	6.300E-03	20	M337	2 1 2 2 1	
3.883E-05	4.358E-03	30.3	M447	0 0 0 0 0	
7.833E-05	8.790E-03	70.4	M447	0 0 0 0 0	
2.511E-04	2.818E-02	100.5	M447	0 0 0 0 0	
6.055E-04	6.795E-02	131.0	M447	0 0 0 0 0	
9.871E-04	1.108E-01	151.2	M447	0 0 0 0 0	
1.633E-03	1.833E-01	170.8	M447	0 0 0 0 0	

1607. $C_8H_{16}Br_2$
1,8-Dibromooctane
Octamethylene dibromide
RN: 4549-32-0 **MP** (°C)**:** 15–16
MW: 272.03 **BP** (°C)**:** 270–272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.389E-06	2.010E-03	1.0	S464	0 0 0 0 0	
7.278E-06	1.980E-03	1.0	S464	0 0 0 0 0	
7.462E-06	2.030E-03	4.9	S464	0 0 0 0 0	
7.646E-06	2.080E-03	4.9	S464	0 0 0 0 0	
8.565E-06	2.330E-03	10.0	S464	0 0 0 0 0	
8.896E-06	2.420E-03	14.9	S464	0 0 0 0 0	
8.528E-06	2.320E-03	14.9	S464	0 0 0 0 0	
9.374E-06	2.550E-03	19.9	S464	0 0 0 0 0	
1.062E-05	2.890E-03	25	S464	0 0 0 0 0	
1.066E-05	2.900E-03	25.0	S464	0 0 0 0 0	
1.044E-05	2.840E-03	25.0	S464	0 0 0 0 0	
1.209E-05	3.290E-03	30.0	S464	0 0 0 0 0	
1.239E-05	3.370E-03	30.0	S464	0 0 0 0 0	
1.213E-05	3.300E-03	30.1	S464	0 0 0 0 0	

(*continued*)

1607. $C_8H_{16}Br_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E-05	3.430E-03	34.9	S464	0 0 0 0 0	
1.309E-05	3.560E-03	35.0	S464	0 0 0 0 0	
1.430E-05	3.890E-03	40.1	S464	0 0 0 0 0	
1.386E-05	3.770E-03	40.1	S464	0 0 0 0 0	

1608. $C_8H_{16}Cl_2$

1,8-Dichlorooctane

RN: 2162-99-4 **MP** (°C)**:** –8
MW: 183.12 **BP** (°C)**:** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-05	4.470E-03	3.6	S464	0 0 0 0 0	
3.047E-05	5.580E-03	5.1	S464	0 0 0 0 0	
3.014E-05	5.520E-03	5.1	S464	0 0 0 0 0	
3.069E-05	5.620E-03	9.9	S464	0 0 0 0 0	
3.233E-05	5.920E-03	15.1	S464	0 0 0 0 0	
3.211E-05	5.880E-03	25.1	S464	0 0 0 0 0	
3.255E-05	5.960E-03	25.1	S464	0 0 0 0 0	
3.222E-05	5.900E-03	25.1	S464	0 0 0 0 0	
3.517E-05	6.440E-03	30.3	S464	0 0 0 0 0	
3.375E-05	6.180E-03	30.3	S464	0 0 0 0 0	
3.823E-05	7.000E-03	35.2	S464	0 0 0 0 0	
3.828E-05	7.010E-03	35.3	S464	0 0 0 0 0	
3.970E-05	7.270E-03	40.1	S464	0 0 0 0 0	

1609. $C_8H_{16}N_2O_2$

N,N,N′,N′-Tetramethylsuccinamide
N,N,N′,N′-Tetramethylbutanediamide

RN: 7334-51-2 **MP** (°C)**:**
MW: 172.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.188E+00	5.490E+02	30	K004	1 0 0 0 2	

1610. $C_8H_{16}N_2O_4S_2$

DL-Homocystine
DL-*meso*-Homocystine
Oxidized DL-homocysteine

RN: 870-93-9 **MP** (°C)**:** 264
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.451E-04	2.000E-01	25	D041	1 0 0 0 0	

1611. $C_8H_{16}N_6$
Pentamethylmelamine
1-(Methylamino)-3,5-bis(dimethylamino)-*s*-triazine
RN: 16268-62-5 **MP** (°C)**:** 107.0
MW: 196.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.679E-04	3.295E-02	25	B386	0 0 0 0 0	
1.010E-02	1.982E+00	25	B386	0 0 0 0 0	
1.101E-02	2.160E+00	25	C051	1 2 1 1 2	pH 7

1612. $C_8H_{16}N_6O$
*N*2-Hydroxy-*N*2,*N*4,*N*4,*N*6,*N*6-pentamethylmelamine
1-(Hydroxylamino)-3,5-bis(dimethylamino)-*s*-triazine
RN: 64124-14-7 **MP** (°C)**:** 110.0
MW: 212.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.412E-03	9.365E-01	25	B386	0 0 0 0 0	
4.259E-03	9.040E-01	25	C051	1 2 1 1 2	pH 7

1613. $C_8H_{16}O$
Cyclooctanol
RN: 696-71-9 **MP** (°C)**:** 15
MW: 128.22 **BP** (°C)**:** 106–108 at 22 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.129E-02	6.576E+00	ns	S460	0 0 0 0 0	

1614. $C_8H_{16}O$
1-Octen-3-ol
3-Octenol
Flowtron mosquito attractant
Matsuka alcohol
Vinyl hexanol
RN: 3391-86-4 **MP** (°C)**:**
MW: 128.22 **BP** (°C)**:** 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.557E-02	1.996E+00	25	D425	0 0 0 0 0	

1615. $C_8H_{16}O$
Hexyl methyl ketone
2-Octanone
Octan-2-one
RN: 111-13-7 **MP** (°C)**:** –16.0
MW: 128.22 **BP** (°C)**:** 172.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.276E-02	4.200E+00	0	C423	0 0 0 0 0	
2.574E-02	3.300E+00	4	C423	0 0 0 0 0	
1.716E-02	2.200E+00	10	C423	0 0 0 0 0	
7.013E-03	8.992E-01	20	D052	1 1 0 0 0	
1.014E-02	1.300E+00	25	C435	0 0 0 0 0	

1616. $C_8H_{16}O$
Caprylic aldehyde
Octaldehyde
n-Octanal
RN: 124-13-0 **MP** (°C)**:**
MW: 128.22 **BP** (°C)**:** 163.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.368E-03	5.600E-01	25	A049	1 0 0 0 1	
1.887E-03	2.420E-01	25	L450	0 0 0 0 0	

1617. $C_8H_{16}O_2$
Ethyl hexanoate
Ethyl butyl acetate
Ethyl caproate
Ethyl *n*-hexanoate
Ethyl caproate (Nat. C-6 ethyl ester)
RN: 123-66-0 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.500E-01	0	C423	0 0 0 0 0	
3.606E-03	5.200E-01	4	C423	0 0 0 0 0	
3.952E-03	5.700E-01	10	C423	0 0 0 0 0	
4.507E-03	6.500E-01	25	C435	0 0 0 0 0	
4.467E-03	6.442E-01	ns	S460	0 0 0 0 0	

1618. $C_8H_{16}O_2$
Valproic acid
Vistora
Valporal
Convulex
Depakote
Dalpro
RN: 99-66-1 **MP** (°C)**:** 120–130
MW: 144.22 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.014E-03	1.300E+00	ns	K444	0 0 0 0 0	
1.380E-02	1.991E+00	ns	S460	0 0 0 0 0	

1619. $C_8H_{16}O_2$
2-Ethylhexoic acid
2-Ethyl-1-hexanoic acid
3-Heptanecarboxylic acid
Butylethylacetic acid
RN: 149-57-5 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-02	1.498E+00	25	O011	1 0 1 1 1	

1620. $C_8H_{16}O_2$
3-Hydroxy-2,2,5,5-tetramethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-2,2,5,5-tetramethyl-
RN: 29839-74-5 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.304E-01	9.091E+01	rt	B066	0 2 0 0 1	

1621. $C_8H_{16}O_2$
n-Butyl *n*-butyrate
Butyl butyrate
RN: 109-21-7 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:** 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-03	4.998E-01	20	D052	1 1 0 0 0	

1622. $C_8H_{16}O_2$
Pentyl propionate
Propanoic acid pentyl ester
Amyl *n*-propanoate
n-Pentyl propionate
RN: 624-54-4 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	7.067E-01	20	S006	1 0 0 0 1	

1623. $C_8H_{16}O_2$
3-Hydroxy-2,2-diethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1624. $C_8H_{16}O_2$
sec-Hexyl acetate
Methyl amyl acetate
RN: 108-84-9 **MP** (°C)**:** –64
MW: 144.22 **BP** (°C)**:** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.543E-03	7.994E-01	20	D052	1 1 0 0 0	

1625. $C_8H_{16}O_2$
Isobutyl isobutyrate
Isobutyl 2-methylpropanoate
2-Methylpropyl 2-methylpropanoate
IBIB
RN: 97-85-8 **MP** (°C)**:** –81
MW: 144.22 **BP** (°C)**:** 147

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-03	5.700E-01	25	A049	1 0 0 0 1	

1626. $C_8H_{16}O_2$
3-Hydroxy-2-ethyl-5,5-dimethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5,5-dimethyl-
RN: 29839-59-6 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.302E-01	4.762E+01	rt	B066	0 2 0 0 0	

1627. $C_8H_{16}O_2$
3-Hydroxy-5-ethyl-2,5-dimethyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-2,5-dimethyl-
RN: 29839-60-9 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E+00	5.000E+02	rt	B066	0 2 0 0 2	

1628. $C_8H_{16}O_2$
3-Hydroxy-5-methyl-5-propyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5-methy-5-propyl-
RN: 29839-52-9 **MP** (°C)**:**
MW: 144.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1629. $C_8H_{16}O_2$
Hexyl acetate
2-Ethyl butyl acetate
RN: 142-92-7 **MP** (°C)**:** –80
MW: 144.22 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.158E-03	5.996E-01	20	D052	1 1 0 0 0	
3.540E-03	5.105E-01	25	M124	2 1 2 2 2	

1630. $C_8H_{16}O_2$
Caprylic acid
Caprylsaure
RN: 124-07-2 **MP** (°C)**:** 16.7
MW: 144.22 **BP** (°C)**:** 239.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-03	4.400E-01	0	B136	1 0 2 1 1	
4.993E-03	7.200E-01	15	F300	1 0 0 0 1	
4.715E-03	6.800E-01	20	B136	1 0 2 1 1	
4.712E-03	6.795E-01	20	D041	1 0 0 0 1	
4.712E-03	6.795E-01	20.0	R001	1 1 1 1 1	
5.478E-03	7.900E-01	30	B136	1 0 2 1 1	
5.471E-03	7.890E-01	30	E005	2 1 1 2 2	
5.474E-03	7.894E-01	30.0	R001	1 1 1 1 1	
5.845E-03	8.430E-01	40	E005	2 1 1 2 2	
6.587E-03	9.500E-01	45	B136	1 0 2 1 1	
6.581E-03	9.491E-01	45.0	R001	1 1 1 1 1	
6.539E-03	9.430E-01	50	E005	2 1 1 2 2	
7.835E-03	1.130E+00	60	B136	1 0 2 1 2	
7.426E-03	1.071E+00	60	E005	2 1 1 2 2	
7.827E-03	1.129E+00	60.0	R001	1 1 1 1 2	
1.803E-02	2.600E+00	100	F300	1 0 0 0 1	
3.050E-03	4.398E-01	.0	R001	1 1 1 1 1	

1631. $C_8H_{16}O_3$
n-Butyl β-methoxypropionate
Propanoic acid, 3-methoxy-, butyl ester
RN: 4195-88-4 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.117E-02	9.800E+00	25	R034	0 0 0 0 1	

1632. $C_8H_{16}O_3$
Amyl lactate
n-Pentyl lactate
RN: 6382-06-5 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-02	1.000E+01	25	R006	2 2 0 1 2	

1633. $C_8H_{16}O_3$
Methyl β-*n*-butoxypropionate
Butanoic acid, 3-methoxy-3-oxopropyl ester
RN: 40326-33-8 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.076E-02	8.133E+00	25	R034	0 0 0 0 1	

1634. $C_8H_{16}O_3$
n-Propyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, propyl ester
RN: 14144-34-4 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.466E-02	1.517E+01	25	D002	1 2 1 1 2	

1635. $C_8H_{16}O_3$
Butylcellosolve acetate
Ethylene glycol monobutyl ether acetate
Ektasolve EB acetate
n-Butyl cellosolve acetate
Ethylene glycol mono-*n*-butyl ether acetate
RN: 112-07-2 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.567E-02	8.920E+00	20	D052	1 1 0 0 0	

1636. $C_8H_{16}O_3$
2,2,5,5-Tetramethyltetrahydrofuran-3,4-diol
3,4-Furandiol, tetrahydro-2,2,5,5-tetramethyl-
RN: 29839-67-6 **MP** (°C)**:**
MW: 160.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.674E-01	9.091E+01	rt	B066	0 2 0 0 1	

1637. $C_8H_{16}O_3S$
1,2-Oxathiolane, 5-pentyl-, 2,2-dioxide
1-Octanesulfonic acid, 3-hydroxy-, γ-sultone
RN: 5633-87-4 **MP** (°C)**:**
MW: 192.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.499E-01	20	B058	1 2 0 0 1	
7.938E-02	1.526E+01	100	B058	1 2 0 0 2	

1638. $C_8H_{16}O_4$
Metaldehyde
Acetaldehyde homopolymer
Acetaldehyde tetramer
RN: 9002-91-9 **MP** (°C)**:** 112
MW: 176.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	2.000E-01	17	M161	1 0 0 0 2	

1639. $C_8H_{17}Cl$
1-Chlorooctane
1-Octylchloride
n-Octyl chloride
Octyl chloride
RN: 111-85-3 **MP** (°C)**:** –61
MW: 148.68 **BP** (°C)**:** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E+01	3.375E+03	5.0	S454	0 0 0 0 0	
2.210E+01	3.286E+03	10.0	S454	0 0 0 0 0	
2.260E+01	3.360E+03	9.9	S454	0 0 0 0 0	
2.350E+01	3.494E+03	9.9	S454	0 0 0 0 0	
2.370E+01	3.524E+03	9.9	S454	0 0 0 0 0	
2.540E+01	3.776E+03	19.1	S454	0 0 0 0 0	
2.470E+01	3.672E+03	25.0	S454	0 0 0 0 0	
2.620E+01	3.895E+03	25.1	S454	0 0 0 0 0	
2.580E+01	3.836E+03	25.2	S454	0 0 0 0 0	
2.710E+01	4.029E+03	30.0	S454	0 0 0 0 0	
2.700E+01	4.014E+03	34.8	S454	0 0 0 0 0	
2.800E+01	4.163E+03	35.1	S454	0 0 0 0 0	
2.690E+01	3.999E+03	35.1	S454	0 0 0 0 0	
2.750E+01	4.089E+03	40.0	S454	0 0 0 0 0	

1640. $C_8H_{17}N$
D-Coniine
α-Propylpiperidine
D-Coniin
Coniine
RN: 458-88-8 **MP** (°C)**:** –2
MW: 127.23 **BP** (°C)**:** 166–167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	1.800E+01	19.5	F300	1 0 0 0 1	
7.782E-02	9.901E+00	25	D004	0 0 0 0 0	

1641. $C_8H_{17}NO$
Ethylbutylacetamide
2-Ethylhexanamide
EBD
RN: 4164-92-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.072E-02	4.400E+00	37	H347	0 0 0 0 0	

1642. $C_8H_{17}NO$
Ethylisobutylacetamide
2-Ethyl-4-methylpentanamide
EID
RN: 130482-28-9 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1643. $C_8H_{17}NO$
Caprylylamide
Caprylsaeure-amid
RN: 629-01-6 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.288E-02	4.710E+00	100	F300	1 0 0 0 2	

1644. $C_8H_{17}NO$
Propylisopropylacetamide
2-Isopropyl-2-propylacetamide
2-Isopropylvaleramide
PID
RN: 6098-19-7 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.444E-02	3.500E+00	37	H347	0 0 0 0 0	

1645. $C_8H_{17}NO$
2-Isopropyl-3-methyl-butyramide
3-Methyl-2-(1-methylethyl)butanamide
Diisopropylacetamide
RN: 5440-65-3 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1646. $C_8H_{17}NO$
Dimethylbutylacetamide
2,2-Dimethylhexanamide
DBD
RN: 20923-67-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.374E-02	3.400E+00	ns	H348	0 0 0 0 0	

1647. $C_8H_{17}NO$
Valnoctamide
VCD
Valmethamide
2-Ethyl-3-methyl-pentanamide
RN: 4171-13-5 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.074E-02	8.700E+00	ns	H348	0 0 0 0 0	

1648. $C_8H_{17}NO$
Methylpentylacetamide
2-Methyl-heptanamide
MPD
RN: 4164-91-4 **MP** (°C)**:**
MW: 143.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.957E-02	7.100E+00	37	H347	0 0 0 0 0	

1649. $C_8H_{17}NO_2$
n-Heptyl carbamate
Heptyl carbamate
RN: 4248-20-8 **MP** (°C)**:** 66
MW: 159.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	3.822E-01	37	H006	1 2 2 1 1	

1650. $C_8H_{17}NO_3$
N-Isoamylurethane
RN: **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.329E-02	4.082E+00	20	O021	1 0 0 0 0	

1651. C_8H_{18}
2,3,4-Trimethylpentane
2,3,4-Trojmetylopentan
RN: 565-75-3 **MP** (°C)**:** –110
MW: 114.23 **BP** (°C)**:** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-05	2.340E-03	0	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	K119	1 0 0 0 2	
2.013E-05	2.300E-03	25	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	P051	2 1 1 2 2	
1.191E-05	1.360E-03	25.00	P007	2 1 2 2 2	

1652. C_8H_{18}
3-Methylheptane
3-Metyloheptan
RN: 589-81-1 **MP** (°C)**:** –121
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.539E-05	2.900E-03	23	C332	0 0 0 0 0	
6.933E-06	7.920E-04	25	K119	1 0 0 0 2	
6.933E-06	7.920E-04	25	P051	2 1 1 2 2	
6.933E-06	7.920E-04	25.00	P007	2 1 2 2 2	

1653. C_8H_{18}
Isooctane
2:2:4-Trimethylpentane
RN: 540-84-1 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-05	2.460E-03	0	P003	2 2 2 2 2	
1.226E-05	1.400E-03	20	M337	2 1 2 2 1	
9.980E-06	1.140E-03	25	K119	1 0 0 0 2	
2.136E-05	2.440E-03	25	M001	2 1 2 2 2	
2.136E-05	2.440E-03	25	M002	2 1 2 2 2	
2.136E-05	2.440E-03	25	M130	1 0 0 0 2	
1.795E-05	2.050E-03	25	P003	2 2 2 2 2	
9.980E-06	1.140E-03	25	P051	2 1 1 2 2	
9.980E-06	1.140E-03	25.00	P007	2 1 2 2 2	
7.879E-06	9.000E-04	ns	B170	0 0 0 0 2	
7.500E-05	8.567E-03	ns	J300	0 0 0 0 0	

1654. C_8H_{18}
3,4-Dimethylhexane
RN: 583-48-2 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.998E-06	7.994E-04	ns	S460	0 0 0 0 0	

1655. C_8H_{18}
3-Ethylhexane
Ethyl hexane
RN: 619-99-8 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.076E-06	3.514E-04	ns	S460	0 0 0 0 0	

1656. C_8H_{18}
2,4-Dimethylhexane
RN: 589-43-5 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-05	1.294E-03	ns	S460	0 0 0 0 0	

1657. C_8H_{18}
2,3-Dimethylhexane
2:3-Dimethylhexane
RN: 590-73-8 **MP** (°C)**:**
MW: 114.23 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.751E-06	2.000E-04	ns	B170	0 0 0 0 2	

1658. C_8H_{18}
2-Methylheptane
RN: 592-27-8 **MP** (°C)**:** –109
MW: 114.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-05	3.800E-03	23	C332	0 0 0 0 0	

1659. $C_8H_{18}NO_4PS_2$
Vamidothion
O,O-Dimethyl *S*-2-(1-*N*-methylcarbamoylethylmercapto)ethyl thiophosphate
RN: 2275-23-2 **MP** (°C)**:** 35.5
MW: 287.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E+01	4.000E+03	20	M161	1 0 0 0 0	
1.392E+01	4.000E+03	ns	M061	0 0 0 0 2	

1660. $C_8H_{18}N_2O$
Di-*n*-butylnitrosamine
N-Nitroso-di-*n*-butylamine
Dibutylnitrosamine
RN: 924-16-3 **MP** (°C)**:**
MW: 158.25 **BP** (°C)**:** 234

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.266E+00	24	D083	2 0 0 0 0	
7.574E-03	1.199E+00	rt	I307	0 0 0 0 0	

1661. $C_8H_{18}O$
2-Octanol
sec-Caprylic alcohol
sec-Octyl alcohol
Methyl hexyl carbinol
RN: 123-96-6 **MP** (°C)**:** –38.6
MW: 130.23 **BP** (°C)**:** 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-02	1.508E+00	15	M073	1 0 2 2 2	
8.131E-03	1.059E+00	20	A015	1 2 1 1 2	
8.600E-03	1.120E+00	20	H330	0 0 0 0 0	
3.059E-02	3.984E+00	25	C093	2 1 1 1 0	
9.829E-03	1.280E+00	25	M073	1 0 2 2 2	
7.892E-03	1.028E+00	ns	J300	0 0 0 0 0	

1662. $C_8H_{18}O$
bis(2-Methyl propyl) ether
iso-Butyl ether
Di-isobutyl ether
RN: 628-55-7 **MP** (°C)**:**
MW: 130.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.059E+00	1.379E+02	25	M375	2 2 2 1 1	
1.227E-02	1.597E+00	51	M375	2 2 2 1 1	
1.002E+00	1.304E+02	60	M375	2 2 2 1 1	

1663. $C_8H_{18}O$
DL-2-Octanol
DL-Octanol-(2)
RN: 4128-31-8 **MP** (°C)**:** –31.6
MW: 130.23 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-02	1.500E+00	15	F300	1 0 0 0 1	
9.214E-03	1.200E+00	25	F300	1 0 0 0 1	

1664. $C_8H_{18}O$

2-Ethyl-1-hexanol
Octyl alcohol
Octyl-(2-ethyl hexyl) alcohol
2-Ethyl hexanol
2-Ethylhexanol
2-Ethylhexan-1-ol

RN: 104-76-7 **MP** (°C)**:** –76
MW: 130.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.318E+00	10.2	S307	1 1 0 2 2	
9.586E-03	1.248E+00	19.8	S307	1 1 0 2 2	
4.604E-03	5.996E-01	20	D052	1 1 0 0 0	
6.760E-03	8.804E-01	20	H330	0 0 0 0 0	
9.982E-04	1.300E-01	25	K072	1 0 1 1 1	
7.441E-03	9.691E-01	29.6	S307	1 1 0 2 1	
8.437E-03	1.099E+00	40.1	S307	1 1 0 2 2	
5.678E-03	7.395E-01	50.2	S307	1 1 0 2 1	
6.598E-03	8.593E-01	60.3	S307	1 1 0 2 1	
7.594E-03	9.890E-01	70.1	S307	1 1 0 2 1	
8.284E-03	1.079E+00	80.1	S307	1 1 0 2 2	
8.973E-03	1.169E+00	90.3	S307	1 1 0 2 2	

1665. $C_8H_{18}O$

1-Octanol
Caprylic alcohol
n-Octyl alcohol
n-Octanol

RN: 111-87-5 **MP** (°C)**:** –16
MW: 130.23 **BP** (°C)**:** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-03	4.198E-01	20	A015	1 2 1 1 2	
3.680E-03	4.793E-01	20	H330	0 0 0 0 0	
3.761E-03	4.898E-01	20.5	S307	1 1 0 2 1	
3.236E-03	4.214E-01	20.96	B178	1 1 0 1 2	EFG
3.162E-03	4.118E-01	23.58	B178	1 1 0 1 2	EFG
2.700E-03	3.516E-01	24	H345	0 0 0 0 0	
4.497E-03	5.857E-01	25	B038	1 2 1 1 2	
3.820E-02	4.975E+00	25	C093	2 1 1 1 0	*sic*
1.000E+00	1.302E+02	25	F044	1 0 0 0 0	EFG
1.060E-03	1.380E-01	25	J035	0 0 0 0 0	
3.830E-03	4.988E-01	25	J302	2 1 2 2 2	
3.800E-03	4.949E-01	25	K025	2 2 1 1 2	
4.530E-03	5.900E-01	25	K072	1 0 1 1 1	
3.970E-03	5.170E-01	25	L322	1 1 2 2 1	
4.530E-03	5.900E-01	25	M087	1 1 2 1 1	
4.110E-03	5.353E-01	25	S359	2 1 2 2 2	

(*continued*)

1665. $C_8H_{18}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.671E-03	9.990E-01	30	R067	0 0 0 0 0	
4.911E-03	6.396E-01	30.6	S307	1 1 0 2 1	
3.236E-03	4.214E-01	34.53	B178	1 1 0 1 2	EFG
1.075E-03	1.400E-01	40	J035	0 0 0 0 0	
4.988E-03	6.496E-01	40.1	S307	1 1 0 2 1	
8.054E-03	1.049E+00	50.0	S307	1 1 0 2 2	
3.548E-03	4.621E-01	60	B178	1 1 0 1 2	EFG
6.751E-03	8.792E-01	60.3	S307	1 1 0 2 1	
3.548E-03	4.621E-01	69.31	B178	1 1 0 1 2	EFG
5.908E-03	7.694E-01	70.3	S307	1 1 0 2 1	
6.675E-03	8.692E-01	80.1	S307	1 1 0 2 1	
6.598E-03	8.593E-01	90.3	S307	1 1 0 2 1	
4.514E-03	5.879E-01	ns	L003	0 0 2 1 2	

1666. $C_8H_{18}O$
n-Butyl ether
Butyl ether
Dibutyl ether
RN: 142-96-1 **MP** (°C)**:** –98
MW: 130.23 **BP** (°C)**:** 142.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E-02	1.847E+00	24.80	O005	2 0 2 2 2	
2.700E-03	3.516E-01	25	K012	1 0 0 0 1	
6.138E-03	7.994E-01	25.50	O005	2 0 2 2 0	
1.720E-02	2.240E+00	37	E028	1 0 1 1 2	

1667. $C_8H_{18}O_2$
Ethohexadiol
2-Ethyl-1,3-hexanediol
RN: 94-96-2 **MP** (°C)**:** –40
MW: 146.23 **BP** (°C)**:** 244.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.103E-02	6.000E+00	20	M161	1 0 0 0 0	
2.756E-01	4.031E+01	25	C093	2 1 1 1 1	
2.756E-01	4.031E+01	ns	M061	0 0 0 0 1	

1668. $C_8H_{18}O_4S_2$
Sulfonethylmethane
Trional
RN: 76-20-0 **MP** (°C)**:** 75
MW: 242.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-02	4.975E+00	16	A072	1 0 1 0 1	
2.063E-02	5.000E+00	16	F300	1 0 0 0 0	
2.042E-02	4.948E+00	ns	R427	0 0 0 0 0	

1669. $C_8H_{19}N$
Octylamine
1-Aminooctane
1-Octanamine
Monoctylamine
n-Octylamine
RN: 111-86-4 **MP** (°C)**:** –5
MW: 129.25 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.547E-03	2.000E-01	25	K072	1 0 1 1 1	
1.547E-03	2.000E-01	25	M087	1 1 2 1 1	

1670. $C_8H_{19}N$
n-Dibutylamine
Di-*n*-butylamine
N,N-Dibutylamine
N-Butyl-1-butanamine
RN: 111-92-2 **MP** (°C)**:** –62
MW: 129.25 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.231E+00	25	K012	1 0 0 0 1	

1671. $C_8H_{19}O_2PS_2$
Ethoprop
Ethoprophos
O-Ethyl-*S,S*-dipropylphosphorodithioate
Holdem
Rovokil
Ethyl *S,S*-dipropyl phosphorodithioate
RN: 13194-48-4 **MP** (°C)**:**
MW: 242.34 **BP** (°C)**:** 88.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.095E-03	7.500E-01	ns	M161	0 0 0 0 2	
3.097E-03	7.506E-01	ns	S460	0 0 0 0 0	

1672. $C_8H_{19}O_2PS_3$
Disulfoton
Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester
Solvirex
Disyston
Thiodemeton
Ethylthiometon
RN: 298-04-4 **MP** (°C)**:** 108
MW: 274.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.940E-05	1.630E-02	19.50	B169	2 1 1 1 2	
9.111E-05	2.500E-02	20	M061	1 0 0 0 1	
5.888E-05	1.616E-02	ns	S460	0 0 0 0 0	
9.111E-05	2.500E-02	rt	M161	0 0 0 0 1	

1673. $C_8H_{19}O_3P$
Dibutyl hydrogen phosphonate
Di-*n*-butyl phosphite
Dibutoxyphosphine oxide
RN: 1809-19-4 **MP** (°C)**:**
MW: 194.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.759E-02	7.300E+00	25	B070	1 2 0 1 1	

1674. $C_8H_{19}O_3PS_2$
Demetonthione
Thiophosphorsaeure-*O,O*-diaethyl-*O*-[2-(aethylthio)-aethyl]-ester
O,O-Diethyl-*O*-(2-(ethylthio)-ethyl)ester thiophosphoric acid
O,O-Diethyl 2-ethylmercaptoethyl thiophosphate
Systox
Thiolo-demeton
RN: 298-03-3 **MP** (°C)**:**
MW: 258.34 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-04	6.000E-02	20	M061	1 0 0 0 1	
7.742E-03	2.000E+00	rt	M161	0 0 0 0 0	form II
2.323E-04	6.000E-02	rt	M161	0 0 0 0 1	form I
1.277E-02	3.300E+00	rt	M161	0 0 0 0 1	

1675. $C_8H_{19}O_3PS_2$
Demetonthiol
Thiophosphorsaeure-*O,O*-diaethyl-*S*-[2-(aethylthio)-aethyl]-ester
O,O-Diethyl-*S*-(2-(ethylthio)-ethyl)ester thiophosphoric acid
RN: 126-75-0 **MP** (°C)**:**
MW: 258.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.742E-03	2.000E+00	20	F300	1 0 0 0 0	

1676. $C_8H_{19}O_4P$
Diethyl butyl phosphate
Butyl diethyl phosphate
RN: 2737-00-0 **MP** (°C)**:**
MW: 210.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.136E-02	1.500E+01	25	B070	1 2 0 1 1	

1677. $C_8H_{19}O_4P$
Diethyl isobutyl phosphate
Ethyl isobutyl phosphate
Phosphoric acid, diethyl 2-methylpropyl ester
RN: 26628-97-7 **MP** (°C)**:**
MW: 210.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-02	1.400E+01	25	B070	1 2 0 1 1	

1678. $C_8H_{19}O_4PS_3$
Disulfoton sulfone
Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester
Disulfoton dioxide
Diethyl *S*-(2-ethylsulfonylethyl) phosphorodithioate
Disyston sulfone
Thiodemeton sulfone
RN: 2497-06-5 **MP** (°C)**:**
MW: 306.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.716E-03	8.323E-01	20	B169	2 2 1 1 1	

1679. $C_8H_{20}Si$
Tetraethylsilicane
Tetraethylsilane
Tetraethylsilicon
RN: 631-36-7 **MP** (°C)**:**
MW: 144.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E-06	3.248E-04	25	D346	0 0 0 0 0	

1680. $C_8H_{20}Sn$
Tetraethyltin
Tetraethylstannane
RN: 597-64-8 **MP** (°C)**:** –112
MW: 234.94 **BP** (°C)**:** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-06	2.678E-04	25	D346	1 1 2 2 2	

1681. $C_8H_{20}O_5P_2S_2$
Sulfotepp
Pirofos
Tetraethyl dithiopyrophosphate
RN: 3689-24-5 **MP** (°C)**:**
MW: 322.32 **BP** (°C)**:** 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.307E-05	3.000E-02	20	F300	1 0 0 0 0	
7.756E-05	2.500E-02	20	M061	1 0 0 0 1	
7.756E-05	2.500E-02	rt	M161	0 0 0 0 1	

1682. $C_8H_{23}N_5$
Tetraethylenepentamine
1,4,7,10,13-Pentaazatridecane
N-(2-Aminoethyl)-*N′*-(2-((2-aminoethyl)amino)ethyl)-1,2-ethanediamine
1,11-Diamino-3,6,9-triazaundecane
3,6,9-Triaza-1,11-undecanediamine
3,6,9-Triazaundecane-1,11-diamine
RN: 112-57-2 **MP** (°C)**:** –40
MW: 189.31 **BP** (°C)**:** 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.582E+00	8.674E+02	4.50	C022	1 2 0 0 2	

1683. $C_8Cl_4N_2$
Chlorothalonil
2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile
Forturf
Exotherm
Bravo
RN: 1897-45-6 **MP** (°C)**:** 250.5
MW: 265.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.256E-06	6.000E-04	25	M161	1 0 0 0 0	

1684. $C_9H_4Cl_3NO_2S$
Folpet
N-(Trichloromethylthio)phthalimide
Folpan
Folpel
Phaltan
Phalton
RN: 133-07-3 **MP** (°C)**:** 177
MW: 296.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-06	1.005E-03	20	B179	0 0 0 0 0	
3.372E-06	1.000E-03	20	F311	1 2 2 2 1	
3.388E-06	1.005E-03	ns	R427	0 0 0 0 0	

1685. $C_9H_5Cl_3N_4$
Anilazine
4,6-Dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine
Triasyn
Direx
Dyrene
Kemate
RN: 101-05-3 **MP** (°C)**:** 159.5
MW: 275.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.629E-05	1.000E-02	ns	B160	0 0 0 0 1	

1686. $C_9H_6ClNO_3S$
Benazolin
7-Chloro-2-oxo-3(2H)-benzothiazolacetic acid
Galipan
Herbazolin
Leymin
Metizolin
RN: 3813-05-6 **MP** (°C)**:** 193
MW: 243.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	6.000E-01	20	M161	1 0 0 0 2	

1687. $C_9H_6Cl_2N_2O_3$
Methazole
2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione
Tunic
Paxilon
Chlormethazole
Mezopur
RN: 20354-26-1 **MP** (°C)**:** 123
MW: 261.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-06	1.500E-03	24	C105	2 1 2 2 2	
5.746E-06	1.500E-03	25	M161	1 0 0 0 1	
5.746E-06	1.500E-03	25	W314	1 0 0 0 1	

1688. $C_9H_6Cl_6O_3S$
Endosulfan
RN: 115-29-7 **MP** (°C)**:** 209
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.987E-07	3.250E-04	ns	V414	0 0 0 0 0	

1689. $C_9H_6Cl_6O_3S$
α-Endosulfan
5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *endo*-
Endosulfan I
Endosulfan A
Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *endo*-
Thiodan I
RN: 959-98-8 **MP** (°C)**:** 109
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-06	5.099E-04	20	B300	2 0 1 1 2	
1.302E-06	5.300E-04	25	W025	1 0 2 2 2	
4.030E-07	1.640E-04	ns	A069	0 0 0 0 2	
1.253E-06	5.100E-04	ns	V414	0 0 0 0 0	

1690. $C_9H_6Cl_6O_3S$
β-Endosulfan
5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *exo*-
Endosulfan II
Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *exo*-
Thiodan II
RN: 33213-65-9 **MP** (°C)**:** 209
MW: 406.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-06	4.501E-04	20	B300	2 0 1 1 2	
6.881E-07	2.800E-04	25	W025	1 0 2 2 2	
1.720E-07	7.000E-05	ns	A069	0 0 0 0 1	
1.106E-06	4.500E-04	ns	V414	0 0 0 0 0	

1691. $C_9H_6I_3NO_3$
2,4,6-Triiodo-3-acetaminobenzoic acid
Acetrizoic acid
RN: 85-36-9 **MP** (°C)**:**
MW: 556.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-03	1.280E+00	25	L025	1 0 0 0 2	
3.232E-03	1.800E+00	50	L025	1 0 0 0 2	
5.387E-03	3.000E+00	100	L025	1 0 0 0 2	
2.442E-03	1.360E+00	ns	H055	0 0 0 0 0	

1692. $C_9H_6N_2S$
4-Cyanobenzyl isothiocyanate
p-Cyanobenzyl isothiocyanate
Isothiocyanic acid, *p*-cyanobenzyl ester
RN: 3694-48-2 **MP** (°C)**:**
MW: 174.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.575E-02	25	D014	1 0 0 0 1	

1693. $C_9H_6O_2$
Coumarin
Cumarin
1,2-Benzopyrone
2H-1-Benzopyran-2-one
Benzopyran-2-one
Benzopyrone
RN: 91-64-5 **MP** (°C)**:** 70
MW: 146.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.153E-03	8.992E-01	.2	D073	1 1 2 1 0	
8.211E-03	1.200E+00	0	F300	1 0 0 0 1	
1.298E-02	1.896E+00	20	D073	1 1 2 1 1	
1.368E-02	2.000E+00	22.5	G301	0 0 0 0 0	
1.706E-02	2.494E+00	25	I312	0 0 0 0 0	
1.774E-02	2.593E+00	30	D073	1 1 2 1 1	
1.847E-02	2.700E+00	30	F300	1 0 0 0 1	
3.065E-02	4.480E+00	40	D073	1 1 2 1 1	
4.419E-02	6.458E+00	50	D073	1 1 2 1 1	
4.756E-02	6.951E+00	60	D073	1 1 2 1 1	
1.342E-01	1.961E+01	100	I312	0 0 0 0 0	
1.507E-02	2.203E+00	ns	R082	0 0 0 0 0	
6.842E-04	9.999E-02	rt	D021	0 0 1 1 0	*sic*

1694. $C_9H_6O_3$
7-Hydroxycoumarin
Umbelliferone
RN: 93-35-6 **MP** (°C)**:** 230
MW: 162.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	3.110E-01	ns	R082	0 0 0 0 0	

1695. $C_9H_6O_5$
Phthalonic acid
Phthalonsaeure
RN: 528-46-1 **MP** (°C)**:**
MW: 194.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.756E+00	5.350E+02	15	F300	1 0 0 0 2	

1696. $C_9H_6O_6$
Trimesic acid
1,3,5-Benzenetricarboxylic acid
Benzol-tricarbonsaeure-(1,3,5)
RN: 554-95-0 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.808E-02	3.800E+00	16	F300	1 0 0 0 1	
1.252E-01	2.630E+01	23	F300	1 0 0 0 2	

1697. $C_9H_6O_6$
1,2,3-Benzenetricarboxylic acid
Benzol-tricarbonsaeure-(1,2,3)
Hemimellitic acid
RN: 569-51-7 **MP** (°C)**:** 223
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	3.060E+01	19	F300	1 0 0 0 2	

1698. $C_9H_6O_6$
Hydrastic acid
Hydrastsaeure
RN: 490-26-6 **MP** (°C)**:**
MW: 210.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-02	6.000E+00	15	F300	1 0 0 0 1	

1699. $C_9H_7Cl_3O_3$
Trichloroethyl salicylate
Benzoic acid, 2-hydroxy-, 2,2,2-trichloroethyl ester
RN: 56529-85-2 **MP** (°C)**:**
MW: 269.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.081E-03	1.100E+00	37	D009	1 2 1 1 1	0.1N HCl

1700. $C_9H_7Cl_3O_3$
Silvex
2-(2,4,5-Trichlorophenoxy)propionic acid
Fenoprop
Propionic acid, 2(2,4,5-trichlorophenoxy)-
RN: 93-72-1 **MP** (°C)**:** 181.6
MW: 269.51 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	7.088E-02	24.99	N417	0 0 0 0 0	
2.634E-04	7.100E-02	25	B164	1 0 1 1 1	
5.195E-04	1.400E-01	25	B185	0 0 0 0 0	
6.678E-04	1.800E-01	25	B200	1 0 0 0 1	
5.195E-04	1.400E-01	25	L024	1 0 0 0 2	
5.194E-04	1.400E-01	25	M061	1 0 0 0 1	
5.195E-04	1.400E-01	25	M161	1 0 0 0 2	
5.194E-04	1.400E-01	ns	B100	0 0 0 0 1	
5.195E-04	1.400E-01	ns	K138	0 0 0 0 1	

1701. C_9H_7N
Quinoline
Chinolin
1-Azanaphthalene
Benzopyridine
1-Benzazine
Benzo[b]pyridine
RN: 91-22-5 **MP** (°C)**:** –15
MW: 129.16 **BP** (°C)**:** 237.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.730E-02	6.110E+00	20	A050	0 0 0 0 0	
4.913E-02	6.346E+00	20.3	L339	2 0 2 2 2	
4.968E-02	6.417E+00	40.0	L339	2 0 2 2 2	
6.337E-02	8.185E+00	64.8	L339	2 0 2 2 2	
8.136E-02	1.051E+01	80.2	L339	2 0 2 2 2	
1.063E-01	1.373E+01	100.0	L339	2 0 2 2 2	

1702. C_9H_7NO
4-Hydroxyquinoline
4-Hydroxy-chinolin
4-Quinolinol
RN: 611-36-9 **MP** (°C)**:** 201
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-02	4.800E+00	15	F300	1 0 0 0 1	

1703. C_9H_7NO
5-Hydroxyquinoline
5-Quinolinol
RN: 578-67-6 **MP** (°C)**:** 223
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.869E-03	4.165E-01	20	A035	1 0 2 2 1	
2.884E-03	4.187E-01	ns	R427	0 0 0 0 0	

1704. C_9H_7NO
6-Hydroxyquinoline
6-Quinolinol
RN: 580-16-5 **MP** (°C)**:** 192
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.882E-03	9.990E-01	20	A035	1 0 2 2 1	

1705. C_9H_7NO
7-Hydroxyquinoline
7-Quinolinol
RN: 580-20-1 **MP** (°C)**:**
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	4.543E-01	20	A035	1 0 2 2 1	
3.162E-03	4.590E-01	ns	R427	0 0 0 0 0	

1706. C_9H_7NO
8-Hydroxyquinoline
8-Quinolinol
Hydroxybenzopuridine
RN: 148-24-3 **MP** (°C)**:** 76
MW: 145.16 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-03	5.552E-01	20	A035	1 0 2 2 1	
4.470E-03	6.489E-01	25.2	P024	2 1 1 1 2	
5.380E-03	7.810E-01	30.3	P024	2 1 1 1 2	

1707. C_9H_7NO
Carbostyril
2-Hydroxyquinoline
2-Quinolinol
RN: 59-31-4 **MP** (°C)**:** 199.0
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.244E-03	1.052E+00	20	C035	1 0 2 2 1	

1708. C_9H_7NO
3-Hydroxyquinoline
3-Quinolinol
RN: 580-18-7 **MP** (°C)**:**
MW: 145.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-03	5.879E-01	20	A035	1 0 2 2 1	

1709. C_9H_7NOS
m-Acetylphenyl isothiocyanate
3-Acetylphenyl isothiocyanate
RN: 3125-71-1 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-05	8.330E-03	25	K032	2 2 0 1 1	

1710. C_9H_7NOS
p-Acetylphenyl isothiocyanate
4-Acetylphenyl isothiocyanate
RN: 2131-57-9 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-05	1.684E-02	25	D019	1 1 1 1 1	

1711. C_9H_7NOS
Phenacyl thiocyanate
RN: 5399-30-4 **MP** (°C)**:**
MW: 177.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-03	3.494E-01	22	J420	0 0 0 0 0	pH 6.5

1712. $C_9H_7NO_2S$
m-Acetoxyphenyl isothiocyanate
Methyl *m*-isothiocyanobenzoate
RN: 3530-01-6 **MP** (°C)**:**
MW: 193.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-04	5.256E-02	25	K032	2 2 0 1 2	
7.700E-04	1.488E-01	25	K032	2 2 0 1 2	

1713. $C_9H_7NO_5$
2-(Oxalylamino)benzoic acid
Oxanil-carbonsaeure-(2)
Oxanil-*o*-carboxylic acid
RN: 5651-01-4 **MP** (°C)**:**
MW: 209.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.259E-03	1.100E+00	10	F300	1 0 0 0 1	

1714. $C_9H_7N_3S$
Tricyclazole
Methyl-1,2,4-triazolo(3,4-b)benzothiazole
5-Methyl-1,2,4-triazolo[3,4-b]benzothiazole
RN: 41814-78-2 **MP** (°C)**:** 187.5
MW: 189.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-03	1.600E+00	25	M161	1 0 0 0 1	

1715. $C_9H_7N_7O_2S$
Azathioprine
Cytostatics
Imuran
Azatioprin
6-(1-Methyl-*p*-nitro-5-imidazolyl)-thiopurine
Ccucol
RN: 446-86-6 **MP** (°C)**:** 243.5
MW: 277.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-04	1.300E-01	24	N016	0 0 0 0 0	
4.472E-04	1.240E-01	25	N063	1 1 1 1 2	intrinsic
4.689E-04	1.300E-01	25	N063	1 1 1 1 2	
3.607E-05	1.000E-02	ns	K444	0 0 0 0 0	

1716. $C_9H_8Cl_2O_3$
Dichlorprop
Dichloroprop
α-(2,4-Dichlorophenoxy)propionic acid
RN: 120-36-5 **MP** (°C)**:** 117.5
MW: 235.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.489E-03	3.500E-01	20	L024	1 0 0 0 2	
1.489E-03	3.500E-01	20	M161	1 0 0 0 2	
1.490E-03	3.503E-01	24.99	N417	0 0 0 0 0	
3.527E-03	8.290E-01	25	B164	1 0 1 1 2	
3.020E-03	7.100E-01	28	B200	1 0 0 0 1	
1.484E-02	3.488E+00	ns	B100	0 0 0 0 1	

1717. $C_9H_8Cl_2O_3$
Methyl (2,4-Dichlorophenoxy)acetate
2,4-Dichorophenoxyacetic acid methyl ester
RN: 5335-03-5 **MP** (°C)**:**
MW: 235.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.657E-04	1.800E-01	ns	B185	0 0 0 0 0	
5.333E-04	1.254E-01	ns	M120	0 0 1 1 2	

1718. $C_9H_8Cl_3NO_2S$
Captan
N-Trichloromethylthio-4-cyclohexene-1,2-dicarboximide
Vancide 89
Merpan 90
Orthocid-83
Pillarcap
RN: 133-06-2 **MP** (°C)**:** 178
MW: 300.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-06	4.989E-04	20	B179	0 0 0 0 0	
<1.66E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.544E-05	4.642E-03	ns	H322	0 0 0 0 0	
1.660E-06	4.989E-04	ns	R427	0 0 0 0 0	
1.663E-06	5.000E-04	rt	M161	0 0 0 0 0	

1719. $C_9H_8N_2OS$
m-Acetamidophenyl isothiocyanate
3-Acetamidophenyl isothiocyanate
RN: 3137-83-5 **MP** (°C)**:**
MW: 192.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.950E-04	5.671E-02	25	K032	2 2 0 1 2	

1720. $C_9H_8N_4O_6$
Nifurtoinol
3-(Hydroxymethyl)nitrofurantoin
RN: 1088-92-2 **MP** (°C)**:**
MW: 268.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	3.300E-01	22	B154	1 1 1 1 1	0.1M HCl

1721. C_9H_8O
(E)-Cinnamaldehyde
(E)-3-Phenylpropenal;
(2E)-3-Phenyl-2-propenal
(E)-3-Phenylprop-2-enone
(E)-3-Phenylacrolein
(E)-3-Phenylprop-2-enal
RN: 14371-10-9 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:** 250–253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	1.850E+00	25	D407	1 0 2 2 2	

1722. C_9H_8O
Cinnamaldehyde
3-Phenyl-2-propenal
Phenylacrolein
3-Phenyl-2-propenaldehyde
Zimtaldehyde
RN: 104-55-2 **MP** (°C)**:**
MW: 132.16 **BP** (°C)**:** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.348E+00	25	I019	1 0 1 2 2	
9.100E-03	1.203E+00	37	E028	1 0 1 1 1	

1723. $C_9H_8O_2$
trans-Cinnamic acid
trans-3-Phenyl-2-propenoic acid
trans-β-Phenylacrylic acid
(E)-3-Phenyl-2-propenoic acid
RN: 140-10-3 **MP** (°C)**:** 133
MW: 148.16 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-03	2.100E-01	15	M461	0 0 0 0 0	
2.700E-03	4.000E-01	18	F300	1 0 0 0 0	
2.835E-03	4.200E-01	18	M077	1 2 1 1 2	
3.010E-03	4.460E-01	25	C090	1 2 2 2 2	
3.685E-03	5.460E-01	25	M077	1 2 1 1 2	
1.552E-03	2.300E-01	25	M461	0 0 0 0 0	
2.092E-03	3.100E-01	30	M461	0 0 0 0 0	
5.264E-03	7.800E-01	35	M077	1 2 1 1 2	
4.252E-03	6.300E-01	40	M461	0 0 0 0 0	
7.364E-03	1.091E+00	45	M077	1 2 1 1 2	
5.737E-03	8.500E-01	50	M461	0 0 0 0 0	

1724. $C_9H_8O_2$
Atropic acid
Atropasaeure
RN: 492-38-6 **MP** (°C)**:** 106
MW: 148.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.774E-03	1.300E+00	20	F300	1 0 0 0 1	

1725. $C_9H_8O_2$
Cinnamic acid
Phenylacrylic acid
3-Phenylpropenoic acid
2-Propenoic acid, 3-phenyl-
RN: 621-82-9 **MP** (°C)**:** 133
MW: 148.16 **BP** (°C)**:** 261.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.024E-03	2.999E-01	10	M043	1 0 0 0 0	
3.390E-03	5.023E-01	14.3	D061	1 0 0 0 2	
2.642E-03	3.914E-01	16.3	D061	1 0 0 0 2	
2.643E-03	3.916E-01	16.30	B118	1 0 0 0 2	unit assumed
1.515E-02	2.245E+00	20	C092	2 1 0 1 1	*sic*
2.699E-03	3.998E-01	20	M043	1 0 0 0 0	
3.170E-03	4.697E-01	22	E045	2 0 1 1 2	
3.260E-03	4.830E-01	23	E045	2 0 1 1 2	
3.360E-03	4.978E-01	24	E045	2 0 1 1 2	
3.450E-03	5.112E-01	25	E045	2 0 1 1 2	
3.850E-03	5.704E-01	25	K040	1 0 2 1 2	
3.340E-03	4.949E-01	25	L048	1 2 2 1 2	
3.340E-03	4.949E-01	25	L050	2 0 1 2 2	
3.540E-03	5.245E-01	26	E045	2 0 1 1 2	
3.800E-03	5.630E-01	26.4	P043	2 0 1 1 2	
3.630E-03	5.378E-01	27	E045	2 0 1 1 2	
4.963E-03	7.353E-01	28	D050	1 2 1 2 2	
4.688E-03	6.946E-01	30	B118	1 0 0 0 2	unit assumed
4.682E-03	6.937E-01	30	D061	1 0 0 0 2	
4.047E-03	5.996E-01	30	M043	1 0 0 0 0	
3.959E-02	5.865E+00	100	M043	1 0 0 0 1	

1726. $C_9H_8O_2$
cis-Cinnamic acid
cis-Zimtsaeure
RN: 102-94-3 **MP** (°C)**:**
MW: 148.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.657E-02	6.900E+00	18	F300	1 0 0 0 1	
4.644E-02	6.880E+00	18	M077	1 2 1 1 2	form III, mp 68 C
5.143E-02	7.620E+00	18	M077	1 2 1 1 2	form II, mp 58 C
6.041E-02	8.950E+00	18	M077	1 2 1 1 2	form I, mp 42 C
5.703E-02	8.450E+00	25	M077	1 2 1 1 2	form III, mp 68 C
6.324E-02	9.370E+00	25	M077	1 2 1 1 2	form II, mp 58 C
7.445E-02	1.103E+01	25	M077	1 2 1 1 2	form I, mp 42 C
7.519E-02	1.114E+01	35	M077	1 2 1 1 2	form III, mp 68 C
8.362E-02	1.239E+01	35	M077	1 2 1 1 2	form II, mp 58 C

(*continued*)

1726. $C_9H_8O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.861E-02	1.461E+01	35	M077	1 2 1 1 2	form I, mp 42 C
9.760E-02	1.446E+01	45	M077	1 2 1 1 2	form III, mp 68 C
1.086E-01	1.609E+01	45	M077	1 2 1 1 2	form II, mp 58 C
1.245E-01	1.845E+01	55	M077	1 2 1 1 2	form III, mp 68 C

1727. $C_9H_8O_3$
2-Acetophenone carboxylic acid
Acetophenon-carbonsaeure-(2)
o-Carboxyacetophenone
RN: 577-56-0 **MP** (°C)**:**
MW: 164.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	3.984E+00	rt	H431	0 0 0 0 0	

1728. $C_9H_8O_4$
Homophthalic acid
Homophthalsaeure
RN: 89-51-0 **MP** (°C)**:** 184.5
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-02	4.579E+00	rt	H431	0 0 0 0 0	

1729. $C_9H_8O_4$
Caffeic acid
3,4-Dihydroxy-*trans*-cinnamate
(E)-3-(3,4-Dihydroxyphenyl)-2-propenoic acid
RN: 331-39-5 **MP** (°C)**:** 196 C
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-03	5.500E-01	15	M461	0 0 0 0 0	
5.440E-03	9.800E-01	25	M461	0 0 0 0 0	
6.827E-03	1.230E+00	30	M461	0 0 0 0 0	
1.132E-02	2.040E+00	40	M461	0 0 0 0 0	
1.621E-02	2.920E+00	50	M461	0 0 0 0 0	

1730. $C_9H_8O_4$
4-Methylphthalic acid
RN: 4316-23-8 **MP** (°C)**:** 149
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.211E-02	3.984E+00	rt	H431	0 0 0 0 0	

1731. $C_9H_8O_4$
Aspirin
Acetyl-salicylsaeure
Acetylsalicylic acid
RN: 50-78-2 **MP** (°C)**:** 135
MW: 180.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-02	5.623E+00	4.62	M053	1 0 1 1 0	EFG, 0.1N HCl
1.107E-02	1.995E+00	12.55	M053	1 0 1 1 0	EFG, 0.1N HCl
3.200E-02	5.765E+00	14	O019	1 0 0 1 2	
1.998E-02	3.600E+00	15	E017	1 0 0 0 0	EFG
1.388E-02	2.500E+00	15	F300	1 0 0 0 1	
1.716E-02	3.091E+00	15	H022	1 2 2 2 2	
2.109E-02	3.800E+00	20	E017	1 0 0 0 0	EFG
1.460E-02	2.630E+00	20.96	M053	1 0 1 1 0	EFG, 0.1N HCl
1.769E-02	3.188E+00	22.5	B422	2 0 2 2 2	
2.553E-02	4.600E+00	25	E017	1 0 0 0 0	EFG
2.775E-02	5.000E+00	25	S304	1 2 1 2 2	form IV
2.131E-02	3.840E+00	25	S304	1 2 1 2 2	form I
2.442E-02	4.400E+00	25	S304	1 2 1 2 2	form II
1.890E-02	3.405E+00	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.62, intrinsic
2.500E-02	4.504E+00	30	A065	2 0 2 2 1	
2.831E-02	5.100E+00	30	E017	1 0 0 0 0	EFG
2.387E-02	4.300E+00	30	G042	1 1 1 1 1	0.1N HCl
2.851E-02	5.137E+00	30	H022	1 2 2 2 2	
2.000E-02	3.603E+00	30	L069	1 0 1 1 0	EFG
2.637E-02	4.750E+00	30	S304	1 2 1 2 2	form I
3.275E-02	5.900E+00	30	S304	1 2 1 2 2	form IV
3.108E-02	5.600E+00	30	S304	1 2 1 2 2	form II
3.275E-02	5.900E+00	35	E017	1 0 0 0 0	EFG
2.942E-02	5.300E+00	37	D009	1 2 1 1 1	0.1N HCl
3.219E-02	5.800E+00	37	G042	1 1 1 1 1	0.1N HCl
3.641E-02	6.560E+00	37	G430	0 0 0 0 0	pH 4.5
3.569E-02	6.430E+00	37	K086	1 0 0 0 2	
3.031E-02	5.460E+00	37	M115	2 2 1 1 2	
4.052E-02	7.300E+00	37	S304	1 2 1 2 2	form II
3.830E-02	6.900E+00	37	S304	1 2 1 2 2	form I
4.218E-02	7.600E+00	37	S304	1 2 1 2 2	form IV
3.441E-02	6.200E+00	37	Y421	0 0 0 0 0	

(*continued*)

1731. $C_9H_8O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	6.900E+00	40	E017	1 0 0 0 0	EFG
4.385E-02	7.900E+00	40	S304	1 2 1 2 2	form II
4.218E-02	7.600E+00	40	S304	1 2 1 2 2	form I
4.607E-02	8.300E+00	40	S304	1 2 1 2 2	form IV
4.662E-02	8.400E+00	45	E017	1 0 0 0 0	EFG
4.274E-02	7.700E+00	45	G042	1 1 1 1 1	0.1N HCl
5.551E-02	1.000E+01	49.42	M053	1 0 1 1 0	EFG, 0.1N HCl
4.940E-02	8.900E+00	50	G042	1 1 1 1 1	0.1N HCl
6.829E-02	1.230E+01	60.17	M053	1 0 1 1 0	EFG, 0.1N HCl
1.848E-02	3.330E+00	ns	K444	0 0 0 0 0	
1.551E-02	2.795E+00	rt	R431	0 0 0 0 0	Average

1732. $C_9H_9ClO_3$

DL-2-(2-Chlorophenoxy)propionic acid
2-(*o*-Chlorophenoxy)propionic acid
3-CP

RN: 76466-16-5 **MP** (°C)**:** 113
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.974E-03	1.199E+00	22	B200	1 0 0 0 1	
9.726E-02	1.951E+01	100	B200	1 0 0 0 2	

1733. $C_9H_9ClO_3$

DL-2-(4-Chlorophenoxy)propionic acid

RN: 3307-39-9 **MP** (°C)**:**
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.352E-03	1.475E+00	25	B164	1 0 1 1 2	
7.352E-03	1.475E+00	25	B185	0 0 0 0 0	

1734. $C_9H_9ClO_3$

(4-Chloro-2-methylphenoxy)acetic acid
MCPA

RN: 94-74-6 **MP** (°C)**:** 120.0
MW: 200.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	6.296E-01	20	M061	1 0 0 0 1	
5.852E-03	1.174E+00	25	B164	1 0 1 1 2	
5.852E-03	1.174E+00	25	B185	0 0 0 0 0	
7.975E-03	1.600E+00	25	B185	0 0 0 0 0	

(*continued*)

1734. $C_9H_9ClO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.979E-03	9.990E-01	ns	B100	0 0 0 0 0	
3.190E-03	6.400E-01	ns	B185	0 0 0 0 0	
4.112E-03	8.250E-01	ns	L024	0 0 0 0 2	
4.112E-03	8.250E-01	rt	M161	0 0 0 0 2	

1735. $C_9H_9Cl_2NO$

Propanil
3′,4′-Dichloropropionanilide
DPA

RN: 709-98-8 **MP** (°C)**:** 85
MW: 218.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.961E-04	1.300E-01	20	F311	1 2 2 2 1	
2.293E-03	5.000E-01	ns	B185	0 0 0 0 0	
2.292E-03	4.998E-01	ns	B200	0 0 0 0 0	
2.293E-03	5.000E-01	ns	H042	0 0 0 0 2	
1.032E-03	2.250E-01	rt	M161	0 0 0 0 2	

1736. $C_9H_9Cl_2NO_2$

Dichlormate
3,4-Dichlorobenzyl *N*-methylcarbamate
Romate

RN: 1966-58-1 **MP** (°C)**:** 52
MW: 234.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	25	B200	1 0 0 0 2	

1737. $C_9H_9Cl_2NO_2$

UC 22463
Sirmate 4E
Rowmate
Sirmate

RN: 62046-37-1 **MP** (°C)**:** 52
MW: 234.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	ns	H042	0 0 0 0 2	

1738. $C_9H_9I_2NO_3$
L-3,5-Diiodotyrosine
3,5-Diiodo-L-tyrosine
DIT
RN: 300-39-0 **MP** (°C)**:** 213
MW: 432.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-03	6.196E-01	25	D041	1 0 0 0 1	

1739. $C_9H_9I_2NO_3$
3,5-Diiodotyrosine
3,5-Diiod-DL-tyrosin
DL-Thyronin
RN: 66-02-4 **MP** (°C)**:** 204
MW: 432.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-03	4.500E-01	15	F300	1 0 0 0 1	
7.850E-04	3.399E-01	25	D041	1 0 0 0 1	
1.386E-03	6.000E-01	25	F300	1 0 0 0 0	
1.316E-02	5.700E+00	75	F300	1 0 0 0 1	

1740. C_9H_9N
Skatole
3-Methyl-indol
3-Methylindole
RN: 83-34-1 **MP** (°C)**:** 95
MW: 131.18 **BP** (°C)**:** 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-03	4.500E-01	16	F300	1 0 0 0 0	

1741. C_9H_9NOS
m-Ethoxyphenyl isothiocyanate
3-Ethoxyphenyl isothiocyanate
RN: 3701-44-8 **MP** (°C)**:**
MW: 179.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-04	6.811E-02	25	K032	2 2 0 1 2	

1742. C_9H_9NOS
p-Ethoxyphenyl isothiocyanate
4-Ethoxyphenyl isothiocyanate
RN: 25687-50-7 **MP** (°C)**:**
MW: 179.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	9.858E-03	25	D019	1 1 1 1 1	

1743. $C_9H_9NO_2$
p-Acetamidobenzaldehyde
Acetamide, *N*-(4-formylphenyl)-
Acetanilide, 4′-formyl-
Micotiazone
RN: 122-85-0 **MP** (°C)**:**
MW: 163.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-02	3.247E+00	25	D044	0 0 0 0 0	

1744. $C_9H_9NO_3$
Hippuric acid
Hippursaeure
N-Benzoylglycine
Benzoylaminoacetic acid
RN: 495-69-2 **MP** (°C)**:** 187
MW: 179.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	3.289E+00	20	D041	1 0 0 0 1	
2.177E-02	3.900E+00	20	F300	1 0 0 0 1	
2.050E-02	3.673E+00	25	B028	1 0 0 0 2	
2.048E-02	3.670E+00	25	K053	2 2 2 2 2	
2.095E-02	3.754E+00	25	L048	1 2 2 1 2	
2.095E-02	3.754E+00	25	L050	2 0 1 2 2	
2.048E-02	3.670E+00	25.1	N026	0 0 0 0 0	
3.320E-02	5.949E+00	38	B028	1 0 0 0 2	
2.334E-02	4.182E+00	rt	D021	0 0 1 1 1	

1745. $C_9H_9NO_3$
Acetamide, 2-(benzoyloxy)-
Glycolamide, benzoate
RN: 64649-43-0 **MP** (°C)**:** 121
MW: 179.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.288E-02	4.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
2.288E-02	4.100E+00	22	N317	1 1 2 1 2	

1746. $C_9H_9NO_4$
Benzadox
((Benzoylamino)oxy)acetic acid
Topcide
RN: 5251-93-4 **MP** (°C)**:**
MW: 195.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.069E-02	1.575E+01	ns	B100	0 0 0 0 1	

1747. C_9H_9NS
p-Methylbenzyl isothiocyanate
4-Methylbenzyl isothiocyanate
RN: 3694-46-0 **MP** (°C)**:**
MW: 163.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	2.612E-02	25	D014	1 0 0 0 1	

1748. $C_9H_9N_3OS$
Benzthiazuron
Benzothiazol-2-yl-3-methylurea
N-2-Benzothiazolyl-*N′*-methylurea
Gatnon
RN: 1929-88-0 **MP** (°C)**:**
MW: 207.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-05	1.200E-02	20	M161	1 0 0 0 1	

1749. $C_9H_9N_3O_2$
Carbendazim
1H-Benzimidazol-2-ylcarbamic acid methyl ester
RN: 10605-21-7 **MP** (°C)**:** 302
MW: 191.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-05	5.800E-03	20	A064	1 0 1 1 1	
3.034E-05	5.800E-03	20	M161	1 0 0 0 1	pH 7

1750. $C_9H_9N_3O_2S_2$
Sulfathiazole
Sulphathiazole
*N*1-2-Thiazolyl-
4-Amino-*N*-2-thiazolyl-
RN: 72-14-0 **MP** (°C)**:** 202
MW: 255.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-03	3.600E-01	16	H114	1 0 0 0 1	
1.743E-03	4.450E-01	20	F073	1 2 2 2 2	
1.958E-03	5.000E-01	20	F074	1 0 0 0 2	
4.426E-03	1.130E+00	20	K028	2 1 2 1 2	pH 7.3, form I
1.414E-03	3.610E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.460E-03	6.280E-01	20	K028	2 1 2 1 2	pH 7.3, form II
2.483E-03	6.340E-01	20	K028	2 1 2 1 2	pH 3.8, form I
1.347E-03	3.439E-01	20	L058	1 0 1 1 1	
2.482E-03	6.336E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 200–202 C
1.413E-03	3.609E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 175 C
1.305E-03	3.332E-01	25	F415	0 0 0 0 0	Average
1.461E-03	3.730E-01	25	H005	1 0 1 2 2	average of 4
1.821E-03	4.650E-01	25	K096	1 2 2 2 2	α form
3.290E-03	8.400E-01	25	K096	1 2 2 2 2	β form
1.796E-03	4.586E-01	25	M440	0 0 0 0 0	
1.966E-03	5.020E-01	26	C102	2 0 2 2 2	
2.350E-03	6.000E-01	26	L052	1 0 0 0 0	
2.270E-03	5.796E-01	30	H018	0 0 0 0 0	
4.308E-03	1.100E+00	30	K096	1 2 2 2 2	β form
2.327E-03	5.940E-01	30	K096	1 2 2 2 2	α form
2.544E-03	6.496E-01	30	M046	1 0 0 0 1	
4.460E-03	1.139E+00	30.0	H010	2 2 1 1 2	
3.564E-03	9.100E-01	35	H114	1 0 0 0 1	
3.094E-03	7.900E-01	35	K096	1 2 2 2 2	α form
5.354E-03	1.367E+00	35	K096	1 2 2 2 2	β form
3.760E-03	9.600E-01	37	C102	2 0 2 2 2	
3.564E-03	9.100E-01	37	D084	1 0 1 0 1	
3.678E-03	9.391E-01	37	F072	1 0 0 0 2	

(*continued*)

1750. $C_9H_9N_3O_2S_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-03	9.411E-01	37	F075	1 0 2 2 2	
3.443E-03	8.790E-01	37	K091	1 0 0 0 2	
2.560E-03	6.536E-01	37	K095	2 0 0 0 2	intrinsic
3.838E-03	9.800E-01	37	L091	1 0 0 0 1	pH 5.5
3.721E-03	9.500E-01	37	M057	1 0 0 0 2	pH 5.5
3.799E-03	9.700E-01	37	R044	0 0 0 0 0	
3.756E-03	9.591E-01	37.50	M142	1 0 0 0 1	
3.603E-03	9.200E-01	38	K006	1 0 0 0 2	
6.619E-03	1.690E+00	40	K096	1 2 2 2 2	β form
4.073E-03	1.040E+00	40	K096	1 2 2 2 2	α form
8.284E-03	2.115E+00	45	K096	1 2 2 2 2	β form
5.288E-03	1.350E+00	45	K096	1 2 2 2 2	α form
6.592E-03	1.683E+00	49	K096	1 2 2 2 2	α form
9.964E-03	2.544E+00	49	K096	1 2 2 2 2	β form
1.683E-03	4.298E-01	ns	L044	0 0 0 0 2	
3.467E-03	8.853E-01	ns	R427	0 0 0 0 0	
1.918E-03	4.898E-01	rt	N015	0 0 2 2 2	

1751. C_9H_{10}
Indan
2,3-Dihydroindene
Hydrindane
1H-Indene, 2,3-dihydro-
Hydrindene
RN: 496-11-7 **MP** (°C)**:** –51.4
MW: 118.18 **BP** (°C)**:** 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.232E-04	1.091E-01	25	M064	1 1 2 2 2	
7.522E-04	8.890E-02	25	P051	2 1 1 2 2	
9.232E-04	1.091E-01	ns	M344	0 0 0 0 2	

1752. C_9H_{10}
α-Methylstyrene
2-Phenyl-1-propene
Isopropenylbenzene
2-Phenylpropene
β-Phenylpropene
RN: 98-83-9 **MP** (°C)**:** –24.0
MW: 118.18 **BP** (°C)**:** 167.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-04	1.155E-01	ns	D001	0 0 0 0 2	

1753. $C_9H_{10}BrClN_2O_2$

Chlorbromuron
3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea
N′-(4-Bromo-3-chlorophenyl)-*N*-methoxy-*N*-methylurea
Maloran
RN: 13360-45-7 **MP** (°C)**:**
MW: 293.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.529E-02	20	B179	0 0 0 0 0	
1.192E-04	3.500E-02	20	M161	1 0 0 0 1	
1.703E-04	5.000E-02	ns	B200	0 0 0 0 1	
1.703E-04	5.000E-02	ns	G036	0 0 0 0 1	

1754. $C_9H_{10}Cl_2N_2O$

Diuron
1,1-Dimethyl-3-(3,4-dichlorophenyl)urea
3-(3,4-Dichlorophenyl)-1,1-dimethylurea
RN: 330-54-1 **MP** (°C)**:** 158
MW: 233.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	4.242E-02	20	B179	0 0 0 0 0	
9.438E-05	2.200E-02	20	E048	1 2 1 1 1	
1.716E-04	4.000E-02	25	A039	1 1 0 0 2	
1.802E-04	4.200E-02	25	B185	0 0 0 0 0	
1.802E-04	4.200E-02	25	B200	1 0 0 0 1	
1.802E-04	4.200E-02	25	G036	1 0 0 0 1	
1.802E-04	4.200E-02	25	G099	1 0 0 1 0	
1.600E-04	3.730E-02	25	H073	2 1 1 2 2	
1.802E-04	4.200E-02	25	M061	1 0 0 0 1	
1.802E-04	4.200E-02	25	M161	1 0 0 0 1	
1.802E-04	4.200E-02	25	N333	0 0 0 0 0	
1.716E-04	4.000E-02	ns	B160	0 0 0 0 1	
1.802E-04	4.200E-02	ns	H042	0 0 0 0 1	
1.000E+02	2.331E+04	ns	H342	0 0 0 0 0	EFG, *sic*
1.802E-04	4.200E-02	ns	K007	0 0 0 0 1	
1.995E-04	4.651E-02	ns	M163	0 0 0 0 0	EFG
1.802E-04	4.200E-02	ns	V414	0 0 0 0 0	

1755. $C_9H_{10}Cl_2N_2O_2$

Linuron
3-(3,4-Dichlorophenyl)-1-methoxy-1-methylurea
RN: 330-55-2 **MP** (°C)**:** 93
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-04	7.523E-02	20	B179	0 0 0 0 0	
3.011E-04	7.500E-02	25	B185	0 0 0 0 0	

(*continued*)

1755. $C_9H_{10}Cl_2N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-04	7.500E-02	25	B200	1 0 0 0 1	
3.011E-04	7.500E-02	25	M061	1 0 0 0 1	
3.011E-04	7.500E-02	25	M161	1 0 0 0 1	
3.252E-04	8.100E-02	25	M162	1 1 0 0 1	
3.011E-04	7.500E-02	ns	K007	0 0 0 0 1	

1756. $C_9H_{10}Cl_2O$

2,4-Dichloro-6-propyl-phenol
RN: 91399-12-1 **MP** (°C)**:**
MW: 205.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.005E-01	25	B316	0 0 0 0 0	

1757. $C_9H_{10}Cl_3O_3PS$

Trichlormetafos-3
O-Methyl *O*-ethyl *O*-2,4,5-trichlorophenyl thiophosphate
RN: 2633-54-7 **MP** (°C)**:**
MW: 335.58 **BP** (°C)**:** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.19E-04	<4.00E-02	ns	M061	0 0 0 0 0	

1758. $C_9H_{10}NO_3$

2-Oxo-5-indolinyl acetate
5-Acetoxy-2-oxindole
RN: 74973-14-1 **MP** (°C)**:**
MW: 180.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	5.225E+00	25	A066	1 0 1 1 1	

1759. $C_9H_{10}NO_3PS$

Cyanophos
Dimethyl *O*-(*p*-cyanophenyl) phosphorothioate
Ciafos
CYAP
RN: 2636-26-2 **MP** (°C)**:** 14.5
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.891E-04	4.600E-02	30	M161	1 0 0 0 1	

1760. $C_9H_{10}N_2O_2$
Phenacemide
Phenylacetyl urea
RN: 63-98-9 **MP** (°C)**:** 215
MW: 178.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E-03	1.820E-01	ns	B404	0 2 1 1 0	

1761. $C_9H_{10}N_2O_3$
p-Nitroacetotoluide
4-Nitroacetotoluide
RN: **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1762. $C_9H_{10}N_2O_3$
p-Ureidophenyl acetate
4-Ureidophenyl acetate
RN: 59746-11-1 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-03	6.214E-01	25	A066	1 0 1 1 1	

1763. $C_9H_{10}N_2O_3$
o-Nitroacetotoluide
2-Nitroacetotoluide
RN: 612-45-3 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1764. $C_9H_{10}N_2O_3S_2$
Ethoxzolamide
6-Ethoxy-2-benzothiazolesulfonamide
Diuretic C
Cardrase
RN: 452-35-7 **MP** (°C)**:** 188
MW: 258.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.033E-02	25	C415	1 0 0 1 0	
1.548E-04	4.000E-02	ns	M032	0 0 0 0 0	
1.549E-04	4.001E-02	ns	R428	0 0 0 0 0	

1765. $C_9H_{10}N_2S$
4-Dimethylaminophenyl isothiocyanate
4-Isothiocyanato-*N,N*-dimethyl-benzenamine
RN: 2131-64-8 **MP** (°C)**:**
MW: 178.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-05	1.337E-02	25	D019	1 1 1 1 1	

1766. $C_9H_{10}N_2S$
3-Dimethylaminophenyl isothiocyanate
N′,N′-Dimethyl-*m*-aminophenyl isothiocyanate
RN: 2392-67-8 **MP** (°C)**:**
MW: 178.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-04	7.487E-02	25	D019	1 1 1 1 2	
1.950E-04	3.476E-02	25	K032	2 2 0 1 2	

1767. $C_9H_{10}N_4$
2,6,7-Trimethylpteridine
2:6:7-Trimethylpteridine
RN: 23767-00-2 **MP** (°C)**:**
MW: 174.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.087E-02	1.235E+01	20	A083	1 2 0 0 0	

1768. $C_9H_{10}N_4O_2S_2$
Sulfamethizole
Sulfamethylthiadiazole
RN: 144-82-1 **MP** (°C)**:** 208
MW: 270.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.957E-03	5.290E-01	20	F073	1 2 2 2 2	
3.320E-03	8.975E-01	37	A046	2 0 1 1 2	
3.884E-03	1.050E+00	37	B046	1 0 2 2 2	pH 4.5
3.270E-03	8.840E-01	37	K091	1 0 0 0 2	
3.270E-03	8.840E-01	37	W016	2 0 1 1 2	
2.938E-03	7.943E-01	ns	N057	1 0 2 2 0	EFG, intrinsic

1769. $C_9H_{10}O$
Propiophenone
1-Phenyl-1-propanone
Ethyl phenyl ketone
Propiophenoe
RN: 93-55-0 **MP** (°C)**:** 19
MW: 134.18 **BP** (°C)**:** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-02	1.985E+00	ns	S460	0 0 0 0 0	

1770. $C_9H_{10}O_2$
Hydrocinnamic acid
Hydrozimtsaeure
RN: 501-52-0 **MP** (°C)**:** 48
MW: 150.18 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.929E-02	5.900E+00	20	F300	1 0 0 0 2	
6.162E-02	9.254E+00	30	D033	2 2 1 2 2	
7.668E-02	1.152E+01	40	D033	2 2 1 2 2	

1771. $C_9H_{10}O_2$
2,5-Dimethylbenzoic acid
2-Carboxy-1,4-dimethylbenzene
Isoxylic acid
RN: 610-72-0 **MP** (°C)**:** 132.5–134.5
MW: 150.18 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-03	1.800E-01	25	H007	0 0 0 0 0	

1772. $C_9H_{10}O_2$
2,4-Dimethylbenzoic acid
4-Carboxy-1,3-dimethylbenzene
RN: 611-01-8 **MP** (°C)**:** 124–126
MW: 150.18 **BP** (°C)**:** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.065E-03	1.600E-01	25	H007	0 0 0 0 0	

1773. $C_9H_{10}O_2$
Benzyl acetate
Phenylmethyl acetate
Acetic acid phenylmethyl ester
α-Acetoxytoluene
RN: 140-11-4 **MP** (°C)**:** –51.3
MW: 150.18 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.973E-03	1.498E+00	25	M350	1 0 1 1 1	

1774. $C_9H_{10}O_2$
3,4-Dimethylbenzoic acid
1-Carboxy-3,4-dimethylbenzene
RN: 619-04-5 **MP** (°C)**:** 165
MW: 150.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-04	1.292E-01	ns	C014	0 0 0 1 1	

1775. $C_9H_{10}O_2$
Ethyl benzoate
Ethyl *p*-benzoate
Benzoesaeure-aethyl ester
RN: 93-89-0 **MP** (°C)**:** –34
MW: 150.18 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.990E-03	1.200E+00	22	N317	1 1 2 1 2	
4.794E-03	7.200E-01	25	A003	1 2 1 2 1	
6.659E-03	1.000E+00	60	F300	1 0 0 0 0	

1776. $C_9H_{10}O_3$
4-Hydroxy-3-ethoxybenzaldehyde
Ethylprotal; ethylvanillin
Bourbonal
Ethovan
NSC 67240
Ethavan
RN: 121-32-4 **MP** (°C)**:** 65
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.019E+00	1.693E+02	25	D407	1 0 2 2 2	

1777. $C_9H_{10}O_3$
Ethyl salicylate
Ethyl *o*-hydroxybenzoate
RN: 118-61-6 **MP** (°C)**:** 1–3
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.032E-02	6.700E+00	37	D009	1 2 1 1 1	0.1N HCl

1778. $C_9H_{10}O_3$
Ethylparaben
4-Hydroxybenzoic acid ethyl ester
Ethyl *p*-hydroxybenzoate
Ethyl 4-hydroxybenzoate
RN: 120-47-8 **MP** (°C)**:** 116
MW: 166.18 **BP** (°C)**:** 297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.750E-03	4.570E-01	15	B355	0 0 0 0 0	
3.370E-03	5.600E-01	20	B355	0 0 0 0 0	
4.910E-03	8.159E-01	20	C006	1 2 1 1 2	
5.329E-03	8.855E-01	25	A059	1 0 1 1 1	
4.090E-03	6.797E-01	25	B355	0 0 0 0 0	
4.510E-03	7.494E-01	25	D081	1 2 2 1 2	
5.300E-03	8.807E-01	25	D339	0 0 0 0 0	
6.310E-03	1.049E+00	25	F322	2 0 1 1 0	EFG
9.628E-03	1.600E+00	25	O027	1 0 1 0 1	
6.379E-03	1.060E+00	25	P013	0 0 0 0 0	
9.500E-03	1.579E+00	27	B129	2 2 2 2 1	
5.200E-03	8.641E-01	27	G078	2 1 0 1 0	EFG
5.400E-03	8.974E-01	27.0	G067	2 0 1 1 1	
6.770E-03	1.125E+00	30	A059	1 0 1 1 2	
8.266E-03	1.374E+00	35	A059	1 0 1 1 2	
7.568E-03	1.258E+00	39.3	G302	2 2 2 2 0	EFG
9.540E-03	1.585E+00	40	A059	1 0 1 1 2	

1779. $C_9H_{10}O_3$
Methyl-4-methoxybenzoate
Methyl anisate
RN: 121-98-2 **MP** (°C)**:** 49
MW: 166.18 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-03	6.431E-01	20	C006	1 0 1 1 2	

1780. $C_9H_{10}O_3$
DL-Tropic acid
DL-Tropasaeure
RN: 529-64-6 **MP** (°C)**:** 118.5
MW: 166.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-01	1.950E+01	20	F300	1 0 0 0 2	

1781. $C_9H_{10}O_4$
3,4-Methoxybenzoic acid
Veratrumsaeure
RN: 93-07-2 **MP** (°C)**:**
MW: 182.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-03	5.000E-01	14	F300	1 0 0 0 0	
3.293E-02	6.000E+00	100	F300	1 0 0 0 0	

1782. $C_9H_{11}BrN_2O_2$
Metobromuron
3-(*p*-Bromophenyl)-1-methoxy-1-methylurea
Patoran
N′-(4-Bromophenyl)-*N*-methoxy-*N*-methylurea
Pattonex
RN: 3060-89-7 **MP** (°C)**:**
MW: 259.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E-03	3.338E-01	20	B179	0 0 0 0 0	
1.274E-03	3.300E-01	20	B200	1 0 0 0 2	
1.274E-03	3.300E-01	20	G036	1 0 0 0 2	
1.274E-03	3.300E-01	20	M061	1 0 0 0 1	
1.274E-03	3.300E-01	20	M161	1 0 0 0 2	
1.157E-03	2.999E-01	ns	B100	0 0 0 0 0	

1783. $C_9H_{11}ClN_2O$

Monuron
N′-(4-Chlorophenyl)-*N,N*-dimethyl-urea
1,1-Dimethyl-3-(*p*-chlorophenyl)urea
RN: 150-68-5 **MP** (°C)**:** 170.5
MW: 198.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-03	2.000E-01	18	F035	1 0 0 0 0	
1.175E-03	2.334E-01	20	B179	0 0 0 0 0	
1.007E-03	2.000E-01	20	E048	1 2 1 1 2	
1.007E-03	2.000E-01	20	F311	1 2 2 2 1	
1.158E-03	2.300E-01	25	A039	1 1 0 0 2	
1.158E-03	2.300E-01	25	B185	0 0 0 0 0	
1.158E-03	2.300E-01	25	B200	1 0 0 0 2	
1.158E-03	2.300E-01	25	G036	1 0 0 0 2	
1.158E-03	2.300E-01	25	G099	1 0 0 1 0	
1.319E-03	2.620E-01	25	H073	2 1 1 2 2	
1.158E-03	2.300E-01	25	M061	1 0 0 0 2	
1.158E-03	2.300E-01	25	M161	1 0 0 0 2	
1.007E-03	2.000E-01	ns	B100	0 0 0 0 0	
1.158E-03	2.300E-01	ns	B160	0 0 0 0 2	
9.000E-04	1.788E-01	ns	F184	0 0 0 0 0	
1.158E-03	2.300E-01	ns	H112	0 0 0 0 2	
1.158E-03	2.300E-01	ns	K007	0 0 0 0 2	
1.158E-03	2.300E-01	ns	N013	0 0 0 0 2	

1784. $C_9H_{11}ClN_2O_2$

Monolinuron
3-(4-Chlorophenyl)-1-methoxy-1-methylurea
Arresin
Afesin
Aresin
RN: 1746-81-2 **MP** (°C)**:** 80
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.692E-03	5.777E-01	20	B179	0 0 0 0 0	
4.333E-03	9.300E-01	20	G036	1 0 0 0 2	
2.702E-03	5.800E-01	20	M061	1 0 0 0 2	
2.702E-03	5.800E-01	22.5	G301	0 0 0 0 0	
3.424E-03	7.350E-01	25	M162	1 1 0 0 2	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.702E-03	5.800E-01	rt	M161	0 0 0 0 2	

1785. $C_9H_{11}ClO$

3-Methyl-5-ethyl-4-chloro-phenol
m-Cresol, 4-chloro-5-ethyl-
RN: 1125-66-2 **MP** (°C)**:**
MW: 170.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	3.754E-01	25	B316	0 0 0 0 0	

1786. $C_9H_{11}Cl_2N_3O_4S_2$

Methylchlothiazide
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-1,1-dioxide
6-Chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
RN: 135-07-9 **MP** (°C)**:**
MW: 360.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.388E-04	5.000E-02	rt	A095	0 0 2 2 0	

1787. $C_9H_{11}Cl_3NO_3PS$

Chlorpyrifos
O,O-Diethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate
DOWCO 179
RN: 2921-88-2 **MP** (°C)**:** 41.5
MW: 350.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.284E-06	4.502E-04	10	B324	0 0 0 0 0	
1.284E-06	4.500E-04	10	B324	0 0 0 0 0	
1.997E-06	7.000E-04	19	B169	2 1 1 1 1	
2.082E-06	7.299E-04	20	B300	2 1 1 1 2	
2.082E-06	7.299E-04	20	B324	0 0 0 0 0	
2.082E-06	7.300E-04	20	B324	0 0 0 0 0	
1.141E-06	4.000E-04	23	B096	1 2 0 0 0	
3.195E-06	1.120E-03	24	F179	2 2 2 2 2	
1.141E-06	4.000E-04	24	K069	2 0 0 1 1	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
5.705E-06	2.000E-03	35	M161	1 0 0 0 0	
1.141E-06	4.000E-04	ns	F071	0 1 2 1 0	
8.557E-07	3.000E-04	ns	K138	0 0 0 0 1	
5.705E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG
3.195E-06	1.120E-03	ns	V414	0 0 0 0 0	
5.705E-06	2.000E-03	ns	Y414	0 0 0 0 0	

1788. $C_9H_{11}Cl_3NO_4P$
Chlorpyrifos oxon
Chlorpyrifos oxygen analog
Dursban oxygen analog
DOWCO 180
3,5,6-Trichloro-2-pyridyl diethyl phosphate
RN: 5598-15-2 **MP** (°C)**:**
MW: 334.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-03	5.200E-01	24	K069	2 0 0 1 1	

1789. $C_9H_{11}FN_2O_3$
2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxopentyl)-
RN: 145303-99-7 **MP** (°C)**:**
MW: 214.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	1.071 E+00	22	B416	2 2 1 2 1	

1790. $C_9H_{11}FN_2O_4$
1-Butyryloxymethyl-5-fluorouracil
Butanoic acid, (5-fluoro-3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)methyl ester
RN: 66542-37-8 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.170E-02	9.600E+00	22	B321	0 0 0 0 0	pH 4.0
4.170E-02	9.600E+00	22	B332	1 1 0 0 1	pH 4.0
4.952E-02	1.140E+01	22	M317	1 1 1 1 1	

1791. $C_9H_{11}FN_2O_4$
1-Isobutyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 2-methylpropyl ester
RN: 71759-45-0 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.000E+00	22	B332	1 1 0 0 1	pH 4.0

1792. $C_9H_{11}FN_2O_4$
1-Butyloxycarbonyl-5-fluorouracil
5-Fluoro-1-(butoxycarbonyl)uracil
RN: 85326-32-5 **MP** (°C)**:**
MW: 230.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.563E-02	5.900E+00	22	B332	1 1 0 0 1	pH 4.0

1793. $C_9H_{11}IN_2O_5$
2′-Deoxy-5-iodouridine
Idoxuridine
(+)-5-Iodo-2′-deoxyuridine
Herplex
RN: 54-42-2 **MP** (°C)**:** 165
MW: 354.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.650E+03	2.001E+06	25	N332	0 0 0 0 0	pH 7.4

1794. $C_9H_{11}N$
1,2,3,4-Tetrahydroquinoline
Kusol
THQ
RN: 635-46-1 **MP** (°C)**:** 15–17
MW: 133.19 **BP** (°C)**:** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	1.404E+00	20.3	L339	2 0 2 2 2	
1.386E-02	1.847E+00	40.0	L339	2 0 2 2 2	
1.774E-02	2.362E+00	59.8	L339	2 0 2 2 2	
2.326E-02	3.098E+00	79.6	L339	2 0 2 2 2	
2.988E-02	3.980E+00	100.4	L339	2 0 2 2 2	

1795. $C_9H_{11}NO$
N-Methylacetanilide
Acetamide, *N*-methyl-*N*-phenyl-
RN: 579-10-2 **MP** (°C)**:** 102
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	2.200E+01	20	B101	0 0 0 0 0	
1.673E-01	2.496E+01	25	B101	0 0 0 0 0	
1.908E-01	2.847E+01	30	B101	0 0 0 0 0	
2.166E-01	3.232E+01	35	B101	0 0 0 0 0	
1.122E-01	1.674E+01	ns	R424	0 0 0 0 0	

1796. $C_9H_{11}NO$
p-Aminopropiophenone
4′-Aminopropiophenone
RN: 70-69-9 **MP** (°C)**:** 140
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-03	3.521E-01	37.5	G002	1 1 1 1 2	pH 6.8

1797. $C_9H_{11}NO$
Propionanilide
Propionsaeure-anilid
Propanilide
RN: 620-71-3 **MP** (°C)**:** 106
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-02	1.800E+00	18	F300	1 0 0 0 1	
1.204E-02	1.797E+00	20	B101	0 0 0 0 0	

1798. $C_9H_{11}NO$
Methyl, [3-(acetylamino)phenyl]-
m-Toluidin-*N*-acetat
m-Toluidine-*N*-acetate
RN: 113321-22-5 **MP** (°C)**:**
MW: 149.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.949E-02	4.400E+00	13	F300	1 0 0 0 1	

1799. $C_9H_{11}NO_2$
Phe
(*S*)-(–)-Phenylalanine
(*S*)-Phenylalanine
2-Amino-3-phenylpropanoic acid
Phenylalanine
RN: 63-91-2 **MP** (°C)**:** 283
MW: 165.19 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-02	9.989E+00	0	D018	2 2 2 1 2	
1.174E-01	1.940E+01	0	F300	1 0 0 0 2	
1.740E-01	2.874E+01	15	D349	2 1 1 2 2	
1.515E-01	2.502E+01	20	B032	1 2 2 1 2	
1.770E-01	2.924E+01	20	D349	2 1 1 2 2	

(*continued*)

1799. $C_9H_{11}NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.637E-01	2.705E+01	25	B032	1 2 2 1 2	
1.740E-01	2.875E+01	25	D041	1 0 0 0 2	
1.800E-01	2.973E+01	25	D349	2 1 1 2 2	
1.816E-01	3.000E+01	25	F300	1 0 0 0 1	
1.649E-01	2.724E+01	25	G092	2 1 1 1 1	
1.649E-01	2.724E+01	25	G315	0 0 0 0 0	
1.625E-01	2.684E+01	25	G433	0 0 0 0 0	
1.589E-01	2.625E+01	25	K031	2 1 2 1 2	
1.200E-01	1.982E+01	25	M097	2 2 2 2 2	
1.494E-01	2.468E+01	25	M374	1 0 2 1 2	
2.100E-01	3.469E+01	25	N001	0 0 0 0 0	EFG
1.720E-01	2.841E+01	25	N012	2 0 2 1 2	
1.574E-01	2.601E+01	25	O316	1 0 1 2 2	
1.575E-01	2.601E+01	25	O316	1 0 1 2 2	
1.689E-01	2.790E+01	25.1	N024	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N025	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N026	0 0 0 0 0	
1.649E-01	2.724E+01	25.1	N027	1 1 2 2 2	
1.717E-01	2.837E+01	27	D036	0 0 0 0 0	
1.683E-01	2.780E+01	27	D036	0 0 0 0 0	
1.834E-01	3.030E+01	28	L081	2 1 2 2 2	
1.790E-01	2.957E+01	29.80	B032	1 2 2 1 2	
2.567E-01	4.240E+01	50	F300	1 0 0 0 2	
3.761E-01	6.212E+01	75	D041	1 0 0 0 2	
3.759E-01	6.210E+01	75	F300	1 0 0 0 2	
4.619E-01	7.630E+01	98	M160	2 1 1 1 0	
5.454E-01	9.010E+01	100	F300	1 0 0 0 2	
9.064E-02	1.497E+01	rt	H431	0 0 0 0 0	

1800. $C_9H_{11}NO_2$

4-(Dimethylamino)benzoic acid

4-Dimethylaminobenzoic acid

RN: 619-84-1 **MP** (°C)**:** 242.5

MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	6.608E-02	ns	C014	0 0 0 1 1	

1801. $C_9H_{11}NO_2$
p-Methoxyacetanilide
p-Acetanisidine
N-(4-Methoxyphenyl)acetamide
N-(4-Methoxyphenyl)acetic acid amide
p-Acetanisidide
Acetamide, *N*-(4-methoxyphenyl)-
RN: 51-66-1 **MP** (°C)**:** 400.3
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.029E-02	1.700E+00	15	F300	1 0 0 0 1	
8.820E-03	1.457E+00	15	M352	1 1 1 1 2	
7.090E-02	1.171E+01	25	D044	0 0 0 0 0	
1.353E-02	2.234E+00	25	M352	1 1 1 1 2	
2.131E-02	3.521E+00	40	M352	1 1 1 1 2	
3.249E-02	5.367E+00	50	M352	1 1 1 1 2	

1802. $C_9H_{11}NO_2$
2-Methyl-4-acetaminophenol
3-Methyl-4-hydroxyacetanilide
3-Methylparacetamol
RN: 16375-90-9 **MP** (°C)**:**
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	4.189E+00	25	D078	1 2 1 1 2	

1803. $C_9H_{11}NO_2$
DL-Phenylalanine
DL-Phenylalanin
RN: 150-30-1 **MP** (°C)**:** 166.5
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.993E-02	9.900E+00	0	F300	1 0 0 0 1	
9.080E-02	1.500E+01	21	F300	1 0 0 0 1	
9.008E-02	1.488E+01	21	P045	1 0 2 1 2	
8.464E-02	1.398E+01	25	D018	2 2 2 1 2	
8.476E-02	1.400E+01	25	D041	1 0 0 0 2	
1.304E-01	2.154E+01	50	D018	2 2 2 1 2	
1.295E-01	2.140E+01	50	F300	1 0 0 0 2	
2.158E-01	3.564E+01	75	D018	2 2 2 1 2	
2.164E-01	3.575E+01	75	D041	1 0 0 0 2	
2.167E-01	3.580E+01	75	F300	1 0 0 0 2	
3.898E-01	6.440E+01	100	F300	1 0 0 0 2	

1804. $C_9H_{11}NO_2$
m-Tolyl methylcarbamate
3-Tolyl methylcarbamate
RN: 1129-41-5 **MP** (°C)**:** 76.5
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.574E-02	2.600E+00	30	M161	1 0 0 0 1	

1805. $C_9H_{11}NO_2$
D-Phenylalanine
D-α-Aminohydrocinnamic acid
D-α-Amino-β-phenylpropionic acid
D-β-Phenyl-α-aminopropionic acid
D-PHE
RN: 673-06-3 **MP** (°C)**:** 273
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.763E-01	2.913E+01	25	D041	1 0 0 0 0	

1806. $C_9H_{11}NO_2$
Ethyl *p*-aminobenzoate
4-Aminobenzoic acid ethyl ester
Ethyl *p*-aminobenzoic acid
Benzocaine
RN: 94-09-7 **MP** (°C)**:** 89.0
MW: 165.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.308E-03	7.117E-01	15	M352	1 1 1 1 2	
1.513E-02	2.500E+00	20	F300	1 0 0 0 1	
5.800E-03	9.581E-01	25	A418	0 0 0 0 0	
4.840E-03	7.995E-01	25	H008	0 0 0 0 0	
6.493E-03	1.073E+00	25	M352	1 1 1 1 2	
6.216E-03	1.027E+00	25	P303	0 0 0 0 0	
6.980E-03	1.153E+00	30	A418	0 0 0 0 0	
7.930E-03	1.310E+00	30	B071	1 2 1 1 2	
5.150E-03	8.507E-01	30	H018	0 0 0 0 0	
7.500E-03	1.239E+00	30	J018	1 2 0 1 1	0.05N NaOH
7.000E-03	1.156E+00	30	L069	1 0 1 1 0	EFG
7.680E-03	1.269E+00	30	R003	0 0 0 0 0	
8.156E-03	1.347E+00	33	P303	0 0 0 0 0	
8.750E-03	1.445E+00	35	A418	0 0 0 0 0	
1.020E-02	1.685E+00	37	F006	1 1 2 2 2	
1.024E-02	1.692E+00	40	A418	0 0 0 0 0	
1.164E-02	1.924E+00	40	M352	1 1 1 1 2	

(*continued*)

1806. $C_9H_{11}NO_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-02	1.704E+00	40	P303	0 0 0 0 0	
1.701E-02	2.810E+00	50	M352	1 1 1 1 2	
>3.03E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.810E-03	7.946E-01	ns	M066	0 0 0 0 2	
4.810E-03	7.946E-01	rt	B016	0 0 1 1 2	pH 7.4
5.135E-03	8.483E-01	rt	I404	0 0 0 0 0	Average

1807. $C_9H_{11}NO_3$

L-Tyrosine
3-(4-Hydroxyphenyl)-L-alanine
Tyrosine
(*S*)-(–)-Tyrosine
p-Tyrosine
L-Tyrosin

RN: 60-18-4 **MP** (°C)**:** 342dec
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.241E-03	2.249E-01	0	D018	2 2 2 1 2	
1.104E-03	2.000E-01	0	F300	1 0 0 0 0	
2.042E-03	3.700E-01	20	B032	1 2 2 1 2	
2.495E-03	4.520E-01	21	P045	1 0 2 1 2	
2.285E-03	4.140E-01	22	A045	2 0 2 2 2	
2.800E-03	5.073E-01	24.99	C404	2 1 2 2 1	
7.800E-02	1.413E+01	25	C405	2 1 2 2 2	intrinsic zwit
2.642E-03	4.788E-01	25	D018	2 2 2 1 2	
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
2.759E-03	5.000E-01	25	F300	1 0 0 0 0	
2.444E-03	4.428E-01	25	G433	0 0 0 0 0	
2.620E-03	4.747E-01	25	H097	2 2 2 2 2	
2.622E-03	4.750E-01	25.1	N024	0 0 0 0 0	
2.495E-03	4.520E-01	25.1	N025	0 0 0 0 0	
2.489E-03	4.510E-01	25.1	N026	0 0 0 0 0	
2.488E-03	4.508E-01	25.1	N027	1 1 2 2 2	
2.753E-03	4.988E-01	27	D036	0 0 0 0 0	
2.677E-03	4.850E-01	27	D036	0 0 0 0 0	
3.195E-03	5.790E-01	28	L081	2 1 2 2 2	
3.800E-03	6.885E-01	34.99	C404	2 1 2 2 1	
5.050E-03	9.150E-01	44.99	C404	2 1 2 2 1	
6.064E-03	1.099E+00	50	D018	2 2 2 1 2	
6.071E-03	1.100E+00	50	F300	1 0 0 0 1	
1.309E-02	2.372E+00	75	D018	2 2 2 1 2	
1.343E-02	2.434E+00	75	D041	1 0 0 0 2	
1.325E-02	2.400E+00	75	F300	1 0 0 0 1	
3.091E-02	5.600E+00	100	F300	1 0 0 0 1	

1808. $C_9H_{11}NO_3$
D-Tyrosine
3-(4-Hydroxyphenyl)-D-alanine
RN: 556-02-5 **MP** (°C)**:** >300
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
5.789E-03	1.049E+00	50	D041	1 0 0 0 2	

1809. $C_9H_{11}NO_3$
DL-Tyrosine
DL-Tyrosin
3-(4-Hydroxyphenyl)-DL-alanine
DL-2-Amino-3-(4-hydroxyphenyl)-propanoic acid
RN: 556-03-6 **MP** (°C)**:** 325
MW: 181.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.519E-04	1.000E-01	0	F300	1 0 0 0 0	
2.208E-03	4.000E-01	20	F300	1 0 0 0 0	
1.936E-03	3.509E-01	25	D041	1 0 0 0 2	
4.610E-03	8.353E-01	50	D041	1 0 0 0 2	
4.415E-03	8.000E-01	50	F300	1 0 0 0 0	
3.753E-02	6.800E+00	100	F300	1 0 0 0 1	

1810. $C_9H_{11}NO_4$
Dopa
DL-3-(3,4-Dihydroxyphenyl)alanine
DL-Dopa
RN: 63-84-3 **MP** (°C)**:** >270
MW: 197.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	4.975E+00	20	D041	1 0 0 0 0	
1.237E-01	2.439E+01	100	D041	1 0 0 0 1	

1811. $C_9H_{11}NO_4$
Levodopa
L-3,4-Dihydroxyphenylalanin
RN: 59-92-7 **MP** (°C)**:** 277
MW: 197.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	5.000E+00	20	F300	1 0 0 0 0	
1.917E-02	3.780E+00	25	H015	1 0 0 0 2	

(*continued*)

1811. $C_9H_{11}NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.927E-02	3.800E+00	25.1	N025	0 0 0 0 0	
1.268E-01	2.500E+01	100	F300	1 0 0 0 1	
5.071E-03	1.000E+00	ns	K444	0 0 0 0 0	

1812. $C_9H_{11}NS_2Hg$

Phenylmercury dimethyldithiocarbamate
Chipman merbam
Merfenl 51
Phelam DP

RN: 32407-99-1 **MP** (°C)**:** 175
MW: 397.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.508E-05	6.000E-03	20	M161	1 0 0 0 0	

1813. $C_9H_{11}N_3O$

Biacetyl mono(2-pyridyl)-hydrazone
BPH
Biacetyl mono(2-pyridyl)hydrazone

RN: 74158-10-4 **MP** (°C)**:** 95
MW: 177.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.643E-04	9.999E-02	ns	R080	0 0 0 0 0	

1814. $C_9H_{11}N_3O_2S_2$

Sulfathiazoline
Benzenesulfonamide, 4-amino-*N*-(4,5-dihydro-2-thiazolyl)-

RN: 32365-02-9 **MP** (°C)**:**
MW: 257.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-04	1.490E-01	20	F073	1 2 2 2 2	

1815. $C_9H_{11}N_3O_4$

Orotic acid morpholine

RN: **MP** (°C)**:** 289–291
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-01	9.909E+01	–4	N018	0 0 0 0 0	
6.500E-01	1.464E+02	16	N018	0 0 0 0 0	
7.450E-01	1.678E+02	25	N018	0 0 0 0 0	

1816. $C_9H_{11}O_4P$
2-Carboxyethylphenylphosphinic acid
CEPPA
RN: **MP** (°C)**:**
MW: 214.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-02	2.076E+01	25.1	W412	0 0 0 0 0	
1.947E-01	4.171E+01	35.51	W412	0 0 0 0 0	
3.450E-01	7.389E+01	44.92	W412	0 0 0 0 0	
6.388E-01	1.368E+02	54.02	W412	0 0 0 0 0	
1.068E+00	2.287E+02	64.60	W412	0 0 0 0 0	
1.341E+00	2.873E+02	69.60	W412	0 0 0 0 0	
1.536E+00	3.290E+02	71.91	W412	0 0 0 0 0	
1.883E+00	4.034E+02	76.32	W412	0 0 0 0 0	

1817. C_9H_{12}
1,2,3-Trimethylbenzene
Hemimellitene
Hemellitol
RN: 526-73-8 **MP** (°C)**:** –25
MW: 120.20 **BP** (°C)**:** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.450E-04	6.551E-02	25	M342	1 0 1 1 2	
6.256E-04	7.520E-02	25	S005	2 2 2 2 2	
6.256E-04	7.520E-02	25	S191	1 2 2 2 2	
6.256E-04	7.520E-02	25	S358	2 2 2 2 2	

1818. C_9H_{12}
1-Ethyl-2-methylbenzene
2-Ethyltoluene
o-Ethyltoluene
1-Methyl-2-ethylbenzene
RN: 611-14-3 **MP** (°C)**:** –80.8
MW: 120.20 **BP** (°C)**:** 165.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.210E-04	7.464E-02	25	M342	1 0 1 1 2	
7.742E-04	9.305E-02	ns	H123	0 0 0 0 0	

1819. C_9H_{12}
1,8-Nonadiyne
RN: 2396-65-8 **MP** (°C)**:** –21
MW: 120.20 **BP** (°C)**:** 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-03	1.250E-01	25	M001	2 1 2 2 2	

1820. C_9H_{12}
Cumene
Isopropylbenzene
Cumol
2-Phenylpropane
RN: 98-82-8 **MP** (°C)**:** –96
MW: 120.20 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.694E-04	8.046E-02	24.94	G034	1 2 2 2 2	
6.073E-04	7.300E-02	25	A002	1 2 1 1 1	
4.018E-04	4.830E-02	25	K119	1 0 0 0 2	
4.160E-04	5.000E-02	25	M001	2 1 2 2 2	
4.409E-04	5.300E-02	25	M002	2 2 1 2 1	
4.160E-04	5.000E-02	25	M130	1 0 0 0 1	
4.018E-04	4.830E-02	25	P051	2 1 1 2 2	
5.433E-04	6.530E-02	25	S005	2 2 2 2 2	
5.433E-04	6.530E-02	25	S191	1 2 2 2 2	
5.433E-04	6.530E-02	25	S358	2 1 2 2 2	
4.018E-04	4.830E-02	25.00	P007	2 1 2 2 2	
6.897E-04	8.290E-02	29.94	G034	1 2 2 2 2	
7.124E-04	8.563E-02	34.94	G034	1 2 2 2 2	
7.469E-04	8.978E-02	39.94	G034	1 2 2 2 2	
7.867E-04	9.456E-02	44.94	G034	1 2 2 2 2	
8.353E-04	1.004E-01	49.94	G034	1 2 2 2 2	
8.894E-04	1.069E-01	54.94	G034	1 2 2 2 2	
9.566E-04	1.150E-01	59.94	G034	1 2 2 2 2	
1.035E-03	1.243E-01	65.14	G034	1 2 2 2 2	
1.128E-03	1.355E-01	70.34	G034	1 2 2 2 2	
1.226E-03	1.473E-01	75.04	G034	1 2 2 2 2	
1.345E-03	1.617E-01	80.24	G034	1 2 2 2 2	
4.160E-04	5.000E-02	ns	H123	0 0 0 0 0	
4.160E-04	5.000E-02	ns	M344	0 0 0 0 1	

1821. C_9H_{12}
n-Propylbenzene
1-Phenylpropane
Propylbenzene
Isocomene
RN: 103-65-1 **MP** (°C)**:** –99.2
MW: 120.20 **BP** (°C)**:** 159.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-04	5.373E-02	10	O312	2 2 0 2 2	
5.000E-04	6.010E-02	15	F001	1 0 1 2 0	
4.350E-04	5.229E-02	15	O312	2 2 0 2 2	
4.520E-04	5.433E-02	20	O312	2 2 0 2 2	
4.576E-04	5.500E-02	25	A002	1 2 1 1 1	
1.000E-03	1.202E-01	25	K001	1 0 2 1 2	

(*continued*)

1821. C_9H_{12} (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.340E-04	5.217E-02	25	M342	1 0 1 1 2	
4.430E-04	5.325E-02	25	O312	2 2 0 2 2	
8.319E-04	9.999E-02	25	S012	2 0 2 2 1	
4.150E-04	4.988E-02	25	S359	2 1 2 2 2	
3.920E-04	4.712E-02	25	T067	2 1 2 1 2	
4.340E-04	5.217E-02	25	W300	2 2 2 2 2	
4.370E-04	5.253E-02	30	O312	2 2 0 2 2	
4.710E-04	5.661E-02	35	O312	2 2 0 2 2	
5.320E-04	6.394E-02	40	O312	2 2 0 2 2	
5.540E-04	6.659E-02	45	O312	2 2 0 2 2	
1.098E-03	1.320E-01	85.8	G035	1 0 0 0 2	
1.381E-03	1.660E-01	114.5	G035	1 0 0 0 2	
2.670E-03	3.209E-01	140.5	G035	1 0 0 0 2	
7.232E-03	8.692E-01	188.0	G035	1 0 0 0 1	
2.033E-02	2.444E+00	222.0	G035	1 0 0 0 2	
4.576E-04	5.500E-02	ns	H123	0 0 0 0 0	
2.700E-02	3.245E+00	ns	H307	0 0 0 0 0	
4.576E-04	5.500E-02	ns	M344	0 0 0 0 1	

1822. C_9H_{12}
1,2,4-Trimethylbenzene
Pseudocumene
RN: 95-63-6 **MP** (°C)**:** –44
MW: 120.20 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.318E-04	5.190E-02	25	K119	1 0 0 0 2	
4.742E-04	5.700E-02	25	M001	2 1 2 2 2	
4.318E-04	5.190E-02	25	P051	2 1 1 2 2	
4.909E-04	5.900E-02	25	S005	2 2 2 2 2	
4.909E-04	5.900E-02	25	S191	1 2 2 2 2	
4.909E-04	5.900E-02	25	S358	2 1 2 2 2	
4.318E-04	5.190E-02	25.00	P007	2 1 2 2 2	
4.742E-04	5.700E-02	ns	M344	0 0 0 0 1	

1823. C_9H_{12}
p-Ethyltoluene
4-Ethyltoluene
1-Ethyl-4-methylbenzene
RN: 622-96-8 **MP** (°C)**:** –62
MW: 120.20 **BP** (°C)**:** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.891E-04	9.485E-02	ns	H123	0 0 0 0 0	

1824. C_9H_{12}

Mesitylene
1,3,5-Trimethylbenzene
Mesitelene

RN: 108-67-8 **MP** (°C)**:** –44.8
MW: 120.20 **BP** (°C)**:** 164.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.794E-04	4.560E-02	15	S203	1 1 2 1 2	
3.111E-04	3.740E-02	20	M337	2 1 2 2 2	
8.070E-04	9.700E-02	25	A002	1 2 1 1 1	
4.010E-04	4.820E-02	25	S005	2 2 2 2 2	
4.010E-04	4.820E-02	25	S191	1 2 2 2 2	
4.118E-04	4.950E-02	25	S203	1 1 2 1 2	
4.010E-04	4.820E-02	25	S358	2 1 2 2 2	
3.280E-04	3.942E-02	25.04	V013	2 2 2 2 2	
5.322E-04	6.397E-02	29.99	C350	0 0 0 0 0	
4.509E-04	5.420E-02	35	S203	1 1 2 1 2	
5.555E-04	6.677E-02	39.99	C350	0 0 0 0 0	
4.701E-04	5.650E-02	45	S203	1 1 2 1 2	
6.166E-04	7.412E-02	49.99	C350	0 0 0 0 0	
7.555E-04	9.081E-02	59.99	C350	0 0 0 0 0	
9.221E-04	1.108E-01	69.99	C350	0 0 0 0 0	
1.161E-03	1.395E-01	79.99	C350	0 0 0 0 0	
1.361E-03	1.636E-01	89.99	C350	0 0 0 0 0	
1.616E-03	1.943E-01	99.99	C350	0 0 0 0 0	

1825. $C_9H_{12}ClN_5O$

Moxonidine

RN: 75438-57-2 **MP** (°C)**:**
MW: 241.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-03	8.003E-01	ns	R426	0 0 0 0 0	

1826. $C_9H_{12}ClO_2PS_3$

Carbophenothion-methyl
S-p-Chlorophenylthiomethyl *O,O*-dimethyl phosphorodithioate

RN: 953-17-3 **MP** (°C)**:**
MW: 314.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.669E-06	1.470E-03	10	B324	0 0 0 0 0	
4.670E-06	1.470E-03	10	B324	0 0 0 0 0	
5.178E-06	1.630E-03	20	B300	2 1 1 1 2	
5.083E-06	1.600E-03	20	B324	0 0 0 0 0	
5.082E-06	1.600E-03	20	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
3.176E-06	1.000E-03	rt	M161	0 0 0 0 0	

1827. $C_9H_{12}ClO_4P$
Heptenophos
7-Chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl phosphate
Ragadan
Hostaquick
RN: 23560-59-0 **MP** (°C)**:**
MW: 250.62 **BP** (°C)**:** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.975E-03	2.500E+00	23	M161	1 0 0 0 1	

1828. $C_9H_{12}Cl_2N_4$
2,4-Dichloro-6-cyclohexylamino-1,3,5-triazine
2,4-Dichloro-6-(cyclohexylamino)triazine
1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-cyclohexyl-
RN: 27282-86-6 **MP** (°C)**:**
MW: 247.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.046E-04	1.000E-01	ns	B160	0 0 0 0 2	

1829. $C_9H_{12}FN_3O_3$
1-Butylcarbamoyl-5-fluorouracil
N-Butyl-5-fluoro-2,4-dioxo-pyrimidinecarboxamide
RN: 64098-82-4 **MP** (°C)**:** 136
MW: 229.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.577E-03	8.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.577E-03	8.200E-01	22	B388	0 0 0 0 0	

1830. $C_9H_{12}NO_5PS$
Fenitrothion
Dimethyl *O*-(4-nitro-*m*-tolyl) phosphorothioate
Nuvanol
Novathion
Dybar
Metathionine
RN: 122-14-5 **MP** (°C)**:** 3.4
MW: 277.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.089E-05	2.520E-02	20	B169	2 0 1 1 2	
1.396E-04	3.870E-02	22	K137	1 1 2 1 0	*sic*
1.082E-04	3.000E-02	ns	F071	0 1 2 1 1	
1.082E-04	3.000E-02	ns	M061	0 0 0 0 1	
1.082E-04	3.000E-02	ns	M110	0 0 0 0 0	EFG

1831. $C_9H_{12}NO_5PS$

O-Methyl *O*-ethyl *O*-4-nitrophenyl thiophosphate
Ethylmethylthiophos
Methylethylthiophos
Methylethylthiofos

RN: 2591-57-3 **MP** (°C)**:**
MW: 277.24 **BP** (°C)**:** 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-04	4.000E-02	ns	M061	0 0 0 0 1	

1832. $C_9H_{12}N_2O$

Fenuron
3-Phenyl-1,1-dimethylurea
N,N-Dimethyl-*N*-phenylurea
Beet-Klean

RN: 101-42-8 **MP** (°C)**:** 133–134
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-02	3.849E+00	20	B179	0 0 0 0 0	
2.245E-02	3.686E+00	20	E048	1 2 1 1 2	
2.253E-02	3.700E+00	20	F311	1 2 2 2 1	
1.766E-02	2.900E+00	24	B185	0 0 0 0 0	
1.761E-02	2.892E+00	24	M061	1 0 0 0 1	
1.462E-02	2.400E+00	25	A039	1 1 0 0 2	
2.345E-02	3.850E+00	25	B200	1 0 0 0 0	
2.345E-02	3.850E+00	25	G036	1 0 0 0 2	
1.462E-02	2.400E+00	25	G099	1 0 0 1 0	
2.452E-02	4.027E+00	25	H073	2 1 1 2 2	
2.345E-02	3.850E+00	25	M161	1 0 0 0 2	
2.426E-02	3.984E+00	ns	B100	0 0 0 0 0	
1.462E-02	2.400E+00	ns	B160	0 0 0 0 2	
2.345E-02	3.850E+00	ns	B185	0 0 0 0 0	
1.761E-02	2.892E+00	ns	N013	0 0 0 0 1	

1833. $C_9H_{12}N_2O_2$

Dulcin
(4-Ethoxyphenyl)urea
4-Aethoxy-phenylharnstoff

RN: 150-69-6 **MP** (°C)**:** 173
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.714E-03	1.210E+00	21	F300	1 0 0 0 2	
7.214E-03	1.300E+00	45	F300	1 0 0 0 1	
1.110E-01	2.000E+01	100	F300	1 0 0 0 0	
6.928E-03	1.248E+00	c	I314	0 0 0 0 0	
1.088E-01	1.961E+01	h	I314	0 0 0 0 0	

1834. $C_9H_{12}N_2O_2S$
3-Thio-2,4-diazaspiro[5.5]undecane-1,3,5-trione
2,4-Diazaspiro[5.5]undecane-1,5-dione, 3-thioxo-
2,4-Diazaspiro[5.5]undecane-1,3,5-trione, 3-thio
RN: 52-45-9 **MP** (°C)**:**
MW: 212.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	7.323E-02	25	P350	0 0 0 0 0	intrinsic

1835. $C_9H_{12}N_2O_3$
5-Allyl-5-ethylbarbituric acid
Barbituric acid, 5-allyl-5-ethyl
5-Ethyl-5-allylbarbituric acid
Dormitiv
5-Ethyl-5-allylbarbiturate
RN: 2373-84-4 **MP** (°C)**:**
MW: 196.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	4.774E+00	25	P350	0 0 0 0 0	intrinsic

1836. $C_9H_{12}N_2O_3$
2,4-Diazaspiro[5.5]undecane-1,3,5-trione
Spiro[barbituric acid-5,1′-cyclohexane]
Cyclohexane-spirobarbiturate
RN: 52-44-8 **MP** (°C)**:**
MW: 196.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	1.707E-01	25	P350	0 0 0 0 0	intrinsic

1837. $C_9H_{12}N_2O_5$
Deoxyuridine
RN: 951-78-0 **MP** (°C)**:** 168
MW: 228.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	4.685E+02	25.31	T420	0 0 0 0 0	

1838. $C_9H_{12}N_2O_6$
Uridine
RN: 58-96-8 **MP** (°C)**:** 166.5
MW: 244.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.40E+00	~8.30E+02	21.99	T418	0 0 0 0 0	
~3.20E+00	~7.81E+02	22.99	T418	0 0 0 0 0	

1839. $C_9H_{12}N_4O_2$
7-Ethyl theophylline
7-Ethyl-1,3-dimethylxanthine
1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-1,3-dimethyl-
RN: 23043-88-1 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-01	3.665E+01	30	B042	1 2 1 1 2	
1.760E-01	3.665E+01	30	G021	1 0 0 0 2	

1840. $C_9H_{12}N_4O_2$
1-Ethyl theobromine
1-Ethyl-3,7-dimethylxanthine
1H-Purine-2,6-dione, 1-ethyl-3,7-dihydro-3,7-dimethyl-
RN: 39832-36-5 **MP** (°C)**:** 156
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-01	3.977E+01	30	B042	1 2 1 1 2	
1.910E-01	3.977E+01	30	G021	1 0 0 0 2	

1841. $C_9H_{12}N_4O_2$
1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-ethoxyethoxy)-
1-Ethoxyethyl-4-allopurinyl ether
RN: 52717-51-8 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.173E-03	1.910E+00	ns	H067	0 0 0 0 0	

1842. $C_9H_{12}N_4O_2$
8-Methyl caffeine
1,3,7,8-Tetramethylxanthine
RN: 832-66-6 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-02	2.175E+00	20	J009	1 0 2 2 2	

1843. $C_9H_{12}N_4O_3$
7-β-Hydroxyethyltheophylline
1H-Purine-2,6-dione, 3,7-Dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-
Dilaphyllin
Etofylline
Corophyllin-*N*
RN: 519-37-9 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	3.226E+01	ns	J025	0 0 0 0 1	

1844. $C_9H_{12}N_4O_3$
8-Methoxycaffeine
1H-Purine-2,6-dione, 3,7-dihydro-8-methoxy-1,3,7-trimethyl-
RN: 569-34-6 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-02	2.556E+00	25	K008	1 1 0 1 0	EFG
1.115E-04	2.500E-02	rt	N015	0 0 2 2 1	

1845. $C_9H_{12}N_4O_3$
1,3,7,9-Tetramethyluric acid
1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7,9-tetramethyl-
Temorine
Temurin
Ba 2750
RN: 2309-49-1 **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.472E-04	3.300E-02	rt	N015	0 0 2 2 1	

1846. $C_9H_{12}N_4O_3S$
*N*4-Acetylsulfanilylguanidine
Acetamide, *N*-[4-[[(aminoiminomethyl)amino]sulfonyl]phenyl]-
p-(Guanidinosulfonyl)acetanilide
Sulgin ASG
RN: 19077-97-5 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-03	3.998E-01	37.50	M142	1 2 0 0 1	
5.766E-02	1.478E+01	h	M142	0 0 0 0 1	

1847. $C_9H_{12}O$
2,3,5-Trimethyl-phenol
Isopseudocumenol
1-Hydroxy-2,3,5-trimethylbenzene
RN: 697-82-5 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	7.627E-01	25	B316	0 0 0 0 0	

1848. $C_9H_{12}O$
4-Propylphenol
4-Propyphenol
p-*n*-Propylphenol
RN: 645-56-7 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-02	1.427E+00	25	L022	1 0 0 0 0	

1849. $C_9H_{12}O$
2-Propylphenol
2-*n*-Propylphenol
2-Propyphenol
RN: 644-35-9 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.222E-02	1.664E+00	25	L022	1 0 0 0 0	

1850. $C_9H_{12}O$
3-Methyl-5-ethyl-phenol
Phenol, 3-ethyl-5-methyl-
m-Cresol, 5-ethyl-
RN: 698-71-5 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	2.315E+00	25	B316	0 0 0 0 0	

1851. $C_9H_{12}O$
4-Ethyl-3-methylphenol
3-Methyl-4-ethylphenol
4-Ethyl-*m*-cresol
RN: 1123-94-0 **MP** (°C)**:**
MW: 136.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-03	9.990E-01	25	L020	1 0 0 0 0	

1852. $C_9H_{12}O$
2,4,6-Trimethylphenol
2-Hydroxymesitylene
1-Hydroxy-2,4,6-trimethylbenzene
Mesityl alcohol
Hydroxymesitylene
RN: 527-60-6 **MP** (°C)**:** 72
MW: 136.20 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.008E+00	25	B316	0 0 0 0 0	
4.892E-03	6.662E-01	25	L020	1 0 0 0 0	

1853. $C_9H_{12}O_2$
o-Propoxyphenol
2-Propoxyphenol
RN: 6280-96-2 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.359E+00	24.99	B353	0 0 0 0 0	

1854. $C_9H_{12}O_2$
Cumene hydroperoxide
CHP
RN: 80-15-9 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.140E-02	1.391E+01	25	K051	1 2 2 1 2	

1855. $C_9H_{12}O_2$
3-Propoxyphenol
m-Propoxy phenol
Phenol, 3-propoxy-
RN: 16533-50-9 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	3.942E+00	30	B315	0 0 0 0 0	

1856. $C_9H_{12}O_2$
1-*O*-Benzylethanediol
Benzylcellosolve
Benzyl cellosolve
RN: 622-08-2 **MP** (°C)**:**
MW: 152.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.618E-02	3.984E+00	20	D052	1 1 0 0 0	
2.813E-02	4.282E+00	23	M062	1 0 0 0 1	

1857. $C_9H_{13}BrN_2O_2$
5-Bromo-3-*tert*-butyl-6-methyluracil
Compound 733
RN: 7286-76-2 **MP** (°C)**:** 188
MW: 261.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.570E-03	4.100E-01	25	M061	1 0 0 0 0	
3.121E-03	8.150E-01	ns	B185	0 0 0 0 0	

1858. $C_9H_{13}BrN_2O_2$
Bromacil
5-Bromo-6-methyl-3,5-butyluracil
RN: 314-40-9 **MP** (°C)**:** 158.3
MW: 261.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	7.100E-01	25	B200	1 0 0 0 2	
3.119E-03	8.143E-01	25	B200	1 0 0 0 2	
3.121E-03	8.150E-01	25	M061	1 0 0 0 2	
3.121E-03	8.150E-01	25	M161	1 0 0 0 2	
3.061E-03	7.994E-01	ns	B100	0 0 0 0 0	

1859. $C_9H_{13}ClN_2O_2$
Terbacil
3-*tert*-Butyl-5-chloro-6-methyluracil
5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione
Sinbar 80W
Geonter
DPX-D732
RN: 5902-51-2 **MP** (°C)**:** 176.0
MW: 216.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.277E-03	7.100E-01	25	M061	1 0 0 0 2	
3.277E-03	7.100E-01	25	M161	1 0 0 0 2	
3.277E-03	7.100E-01	25	P307	1 0 0 0 1	
3.228E-03	6.995E-01	ns	B100	0 0 0 0 0	

1860. $C_9H_{13}ClN_6$
Cyanazine
Bladex
2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile
Fortrol
Payze
SD 45418
RN: 21725-46-2 **MP** (°C)**:** 166.5
MW: 240.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.647E-04	1.600E-01	23	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	M061	1 0 0 0 2	
7.104E-04	1.710E-01	25	M161	1 0 0 0 2	
6.647E-04	1.600E-01	25	S309	1 0 0 0 2	
8.309E-04	2.000E-01	ns	M110	0 0 0 0 0	EFG

1861. $C_9H_{13}N$
2,4,5-Trimethylaniline
2,4,5-Trimethylanilin
RN: 137-17-7 **MP** (°C)**:**
MW: 135.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.875E-03	1.200E+00	19.40	F300	1 0 0 0 1	
1.109E-02	1.500E+00	28.70	F300	1 0 0 0 1	

1862. $C_9H_{13}NO_3$
Adrenaline
Adrenalin
Epinephrine
L-1-(3,4-Dihydroxyphenyl)-2-methylaminoethanol
Primatene
Epipen
RN: 51-43-4 **MP** (°C)**:**
MW: 183.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.825E-04	1.800E-01	20	F300	1 0 0 0 1	

1863. $C_9H_{13}N_3O_3$
Orotic acid *n*-butylamide
Orotamide, *N*-butyl-
RN: 13156-38-2 **MP** (°C)**:** 276–277
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.204E+01	–4	N018	0 0 0 0 0	
9.600E-02	2.028E+01	16	N018	0 0 0 0 0	
1.180E-01	2.492E+01	25	N018	0 0 0 0 0	

1864. $C_9H_{13}N_3O_3$
Zalcitabine
2′,3′-Dideoxycytidine
Dideoxycytidine
CCRIS 692
Hivid
DDCYD
RN: 7481-89-2 **MP** (°C)**:** 210–214
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.360E-01	7.098E+01	ns	S469	0 0 0 0 0	

1865. $C_9H_{13}N_3O_3$
Orotic acid diethylamine
Orotamide, *N,N*-diethyl-
RN: 883-81-8 **MP** (°C)**:** 192–194
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E+00	6.208E+02	25	N018	0 0 0 0 0	

1866. $C_9H_{13}N_3O_4$
Orotic acid isobutanolamine
RN: **MP** (°C)**:** 247–249
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	9.543E+01	–4	N018	0 0 0 0 0	
7.060E-01	1.604E+02	16	N018	0 0 0 0 0	
8.410E-01	1.911E+02	25	N018	0 0 0 0 0	

1867. $C_9H_{13}N_3O_4$
Cytosine deoxyriboside
RN: 951-77-9 **MP** (°C)**:**
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E+00	6.317E+02	25.23	T420	0 0 0 0 0	

1868. $C_9H_{13}N_3O_5$
Cytidine
RN: 65-46-3 **MP** (°C)**:** > 215
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.70E-01	~2.36E+02	21.99	T418	0 0 0 0 0	
~8.00E-01	~1.95E+02	22.99	T418	0 0 0 0 0	

1869. $C_9H_{13}N_3O_5$
Orotic acid 2-amide-2-methyl-1,3-propanediol
RN: **MP** (°C)**:** 214–215
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-01	8.391E+01	–4	N018	0 0 0 0 0	
5.860E-01	1.425E+02	16	N018	0 0 0 0 0	
6.970E-01	1.695E+02	25	N018	0 0 0 0 0	

1870. $C_9H_{13}N_5O_4$
Ganciclovir
2-Amino-1,9-dihydro-9-((2-hydroxy-1-(hydroxymethyl)ethoxy)methyl)-6H-purin-6-one
DHPG
RN: 82410-32-0 **MP** (°C)**:** 250
MW: 255.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	3.600E+00	25	B360	0 0 0 0 0	
1.230E-02	3.139E+00	25	Z407	0 0 0 0 0	

1871. $C_9H_{13}O_2P$
Mesitylene phosphinous acid
Phosphinic acid, (2,4,6-trimethylphenyl)-
RN: 6781-97-1 **MP** (°C)**:** 147.0
MW: 184.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.882E+00	1	C061	2 2 2 1 2	
1.619E-02	2.981E+00	25	C061	2 2 2 1 2	
1.754E-02	3.230E+00	35	C061	2 2 2 1 2	
2.082E-02	3.835E+00	45	C061	2 2 2 1 2	
2.836E-02	5.223E+00	65	C061	2 2 2 1 2	
3.774E-02	6.951E+00	85	C061	2 2 2 1 2	

1872. $C_9H_{13}O_6PS$
Endothion
O,O-Dimethyl *S*-(5-methoxypyronyl-2-methyl) thiophosphate
RN: 2778-04-3 **MP** (°C)**:** 90.5
MW: 280.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.141E+00	6.000E+02	ns	M061	0 0 0 0 2	
5.353E+00	1.500E+03	ns	M161	0 0 0 0 1	

1873. $C_9H_{14}ClN_5$
Cyprozine
2-Chloro-4-cyclopropylamino-6-isopropylamino-1,3,5-triazine
RN: 22936-86-3 **MP** (°C)**:** 167
MW: 227.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.030E-05	6.900E-03	25	B200	1 0 0 0 1	
8.582E-04	1.954E-01	40	B200	1 0 0 0 2	

1874. $C_9H_{14}N_2O_3$
5-Ethyl-5-*n*-propylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-propyl-
5-Ethyl-5-propylbarbiturate
RN: 33376-25-9 **MP** (°C)**:** 146.5
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.872E-02	5.694E+00	25	B065	1 2 1 1 1	
3.610E-02	7.156E+00	25	M310	2 2 2 2 2	

1875. $C_9H_{14}N_2O_3$
Metharbital
5,5′-Diethyl-1-methylbarbituric acid
RN: 50-11-3 **MP** (°C)**:** 155
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-02	2.000E+00	25	B011	2 0 0 1 0	
9.980E-03	1.978E+00	25	B065	1 1 1 1 1	
1.150E-02	2.280E+00	25	G003	1 1 1 1 2	pH 4.7
6.054E-03	1.200E+00	25	P061	0 0 0 0 0	
4.979E-03	9.870E-01	rt	M161	0 0 0 0 2	

1876. $C_9H_{14}N_2O_3$
Probarbital
5-Ethyl-5-isopropylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylethyl)
RN: 76-76-6 **MP** (°C)**:** 197.5
MW: 198.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.104E-03	1.210E+00	25	B065	1 1 1 1 1	
7.111E-03	1.410E+00	25	P350	0 0 0 0 0	intrinsic
1.210E-01	2.399E+01	40	N008	1 0 1 1 2	*sic*

1877. $C_9H_{14}N_6$
6-Amino-4-(diallylamino)-1,2-dihydro-1-hydroxy-2-imino-*s*-triazine
RN: **MP** (°C)**:**
MW: 206.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-01	3.010E+01	37	H004	0 0 0 0 0	

1878. $C_9H_{14}O_6$
L-Camphoronic acid
L-Camphoronsaeure
RN: 2385-74-2 **MP** (°C)**:**
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.087E-01	1.110E+02	16	F300	1 0 0 0 2	

1879. $C_9H_{14}O_6$
Triacetin
Propane-1,2,3-triyl triacetate
Enzactin
Vanay
Triacetylglycerol
Glycerol triacetate
RN: 102-76-1 **MP** (°C)**:** –78
MW: 218.21 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.290E-01	7.180E+01	15	F300	1 0 0 0 2	
2.389E-01	5.213E+01	24.50	O005	1 0 2 2 1	
3.118E-02	6.803E+00	ns	F014	0 0 0 0 2	

1880. $C_9H_{15}Br_6O_4P$
Tris-BP
tris(2,3-Dibromopropyl) phosphate
2,3-Dibromo-1-propanol phosphate (3:1)
2,3-Dibromopropyl phosphate
Flamex T 23P
Anfram 3PB
RN: 126-72-7 **MP** (°C)**:** 5.5
MW: 697.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.147E-05	8.000E-03	24	H116	2 1 0 0 2	

1881. $C_9H_{15}Cl_6O_4P$
Fyrol FR-2
tris(1,3-Dichloroisopropyl) phosphate
TCPP
Emulsion 212
TDCPP
PF 38
RN: 13674-87-8 **MP** (°C)**:**
MW: 430.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.624E-05	7.000E-03	24	H116	2 1 0 0 2	

1882. $C_9H_{15}NO_3$
Ecgonine
L-Ekgonin
3-Hydroxy-2-tropane carboxylic acid
RN: 481-37-8 **MP** (°C)**:** 198
MW: 185.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.610E-01	1.780E+02	ns	F300	0 0 0 0 2	

1883. $C_9H_{15}NO_3S$
Captopril
1-((2S)-3-mercapto-2-methylpropionyl)-L-proline
Acenorm
Capoten
Capozide
(*S*)-1-(3-Mercapto-2-methyl-1-oxopropyl)-L-proline
RN: 62571-86-2 **MP** (°C)**:**
MW: 217.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.602E-01	1.000E+02	ns	K444	0 0 0 0 0	
6.348E-01	1.379E+02	ns	S469	0 0 0 0 0	

1884. C_9H_{16}
2,2,5-Trimethyl-3-hexyne
3-Hexyne, 2,2,5-trimethyl-
RN: 17530-23-3 **MP** (°C)**:**
MW: 124.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-04	2.994E-02	25	H039	1 2 2 2 2	

1885. C_9H_{16}
1-Nonyne
n-Heptylacetylene
Heptylacetylene
RN: 3452-09-3 **MP** (°C)**:** –50
MW: 124.23 **BP** (°C)**:** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.796E-05	7.200E-03	25	M001	2 1 2 2 1	

1886. $C_9H_{16}ClN_4$
G 30451
2-Chloro-4-propylamino-6-isopropylamino-*s*-triazine
RN: 3567-85-9 **MP** (°C)**:**
MW: 215.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.947E-04	4.200E-02	21	B192	0 0 0 0 1	

1887. $C_9H_{16}ClN_5$
Propazine
2-Chloro-4-isopropylamino-6-isopropylamino-*s*-triazine
RN: 139-40-2 **MP** (°C)**:** 213
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.744E-05	8.600E-03	20	B185	0 0 0 0 0	
4.000E-05	9.189E-03	20	B200	1 0 0 0 0	
2.307E-05	5.300E-03	20	C048	2 2 2 2 1	
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.744E-05	8.600E-03	20	M161	1 0 0 0 1	
3.744E-05	8.600E-03	21	B192	0 0 0 0 1	
3.744E-05	8.600E-03	21	G099	2 0 0 1 0	
3.744E-05	8.600E-03	22	M061	1 0 0 0 1	
7.700E-05	1.769E-02	50	G001	1 0 1 1 1	
3.744E-05	8.600E-03	ns	C101	0 0 0 0 1	
4.353E-05	1.000E-02	ns	G041	0 0 0 0 1	
3.744E-05	8.600E-03	ns	J033	0 0 0 0 0	

1888. $C_9H_{16}ClN_5$
Terbuthylazine
Terbutylazine
2-Chloro-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Primatol M
RN: 5915-41-3 **MP** (°C)**:** 178
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.700E-05	8.500E-03	20	M161	1 0 0 0 1	
3.700E-05	8.500E-03	ns	J033	0 0 0 0 0	

1889. $C_9H_{16}ClN_5$
Trietazine
2-Chloro-4-diethylamino-6-ethylamino-*s*-triazine
2-Chloro-4-ethylamino-6-diethylamino-*s*-triazines
RN: 1912-26-1 **MP** (°C)**:** 101
MW: 229.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.706E-05	2.000E-02	20	B185	0 0 0 0 0	
8.706E-05	2.000E-02	21	B192	0 0 0 0 1	
8.706E-05	2.000E-02	21	G099	2 0 0 1 0	
8.706E-05	2.000E-02	25	M161	1 0 0 0 1	
8.706E-05	2.000E-02	ns	J033	0 0 0 0 0	

1890. $C_9H_{16}N_2O_4$
Methyl-2,2-diethylmalonurate
Methyl 2,2-diethylmalonurate
RN: 69577-07-7 **MP** (°C)**:** 112
MW: 216.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	2.379E+00	23	B152	1 2 1 1 1	pH 3.5

1891. $C_9H_{16}N_4OS$
Tebuthiuron
1-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea
Graslan
Spike
Spike 20P
Perflan
RN: 34014-18-1 **MP** (°C)**:** 162.2
MW: 228.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-02	2.300E+00	ns	M161	0 0 0 0 1	

1892. $C_9H_{16}N_8$
2-Azido-4-ethylamino-4-*t*-butylamino-*s*-triazine
WL 9385
RN: 2854-70-8 **MP** (°C)**:** 102.5
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.047E-04	7.200E-02	20	M061	1 0 0 0 1	

1893. $C_9H_{16}O_2$
3-Hydroxy-5-spirocyclohexyltetrahydrofuran
1-Oxaspiro[4.5]decan-3-ol
RN: 29839-61-0 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-01	1.961E+01	rt	B066	0 2 0 0 0	contains impurity

1894. $C_9H_{16}O_2$
g-Nonanolactone
4-Hydroxynonanoic acid lactone
g-*n*-Amylbutyrolactone
g-Pentyl-g-butyrolactone
g-Nonanolide
RN: 104-61-0 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-02	9.217E+00	25	D407	1 0 2 2 2	
5.902E-02	9.221E+00	ns	S460	0 0 0 0 0	

1895. $C_9H_{16}O_2$
3-Hydroxy-2-methyl-5-spirocyclopentyltetrahydrofuran
1-Oxaspiro[4.4]nonan-3-ol, 2-methyl-
RN: 29839-62-1 **MP** (°C)**:**
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E+00	1.667E+02	rt	B066	0 2 0 0 1	

1896. $C_9H_{16}O_4$
Butyl α-acetoxypropionate
Hydracrylic acid, butyl ester, acetate
RN: 5422-69-5 **MP** (°C)**:**
MW: 188.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.200E+00	25	R006	2 2 0 1 1	

1897. $C_9H_{16}O_4$
Azelaic acid
Azelainsaeure
Nonanedioic acid
RN: 123-99-9 **MP** (°C)**:** 106.5
MW: 188.23 **BP** (°C)**:** 287

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.313E-03	1.000E+00	0	L041	1 0 0 1 1	
3.298E-03	6.208E-01	6.99	A340	0 0 0 0 0	
4.513E-03	8.494E-01	12.69	A340	0 0 0 0 0	
7.969E-03	1.500E+00	15	L041	1 0 0 1 1	
6.475E-03	1.219E+00	18.69	A340	0 0 0 0 0	
1.275E-02	2.400E+00	20	F300	1 0 0 0 1	
1.275E-02	2.400E+00	20	L041	1 0 0 1 1	
1.297E-02	2.441E+00	20	M171	1 0 0 0 1	
2.667E-01	5.020E+01	21	B040	1 0 1 1 2	*sic*
9.461E-03	1.781E+00	24.99	A340	0 0 0 0 0	
1.589E-02	2.990E+00	34.69	A340	0 0 0 0 0	
2.391E-02	4.500E+00	35	L041	1 0 0 1 1	
1.858E-02	3.498E+00	42.99	A340	0 0 0 0 0	
4.356E-02	8.200E+00	50	L041	1 0 0 1 1	
2.662E-02	5.010E+00	52.59	A340	0 0 0 0 0	
3.858E-02	7.263E+00	56.99	A340	0 0 0 0 0	
5.124E-02	9.645E+00	61.49	A340	0 0 0 0 0	
7.023E-02	1.322E+01	64.99	A340	0 0 0 0 0	
1.169E-01	2.200E+01	65	F300	1 0 0 0 1	
1.169E-01	2.200E+01	65	L041	1 0 0 1 1	
7.255E-02	1.366E+01	70.99	A340	0 0 0 0 0	
8.355E-02	1.573E+01	74.49	A340	0 0 0 0 0	
1.048E-01	1.972E+01	79.89	A340	0 0 0 0 0	
9.430E-02	1.775E+01	84.49	A340	0 0 0 0 0	
9.440E-03	1.777E+00	rt	H431	0 0 0 0 0	

1898. $C_9H_{16}O_5$
Propanoic acid, 2-[(butoxycarbonyl)oxy]-, methyl ester
Propanoic acid, 2-[(methoxycarbonyl)oxy]-, butyl ester
RN: **MP** (°C)**:**
MW: 204.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.798E-03	1.797E+00	25	R007	0 0 0 0 0	

1899. $C_9H_{17}ClN_3O_3PS$
Isazophos
Diethyl *O*-(5-chloro-1-(1-methylethyl)-1H-1,2,4-triazol-3-yl) phosphorothioate
Miral
Triumph
CGA-12223
RN: 42509-80-8 **MP** (°C)**:**
MW: 313.74 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.500E-01	20	E048	1 2 1 1 2	
4.781E-04	1.500E-01	20	M161	1 0 0 0 1	

1900. $C_9H_{17}NOS$
Molinate
S-Ethyl hexahydro-1H-azepine-1-carbothioate
Hydram
Carbothialate, ethyl-1-hexa-methylene imine-
Poperidinecarbothioic acid, *S*-ethyl ester
RN: 2212-67-1 **MP** (°C)**:**
MW: 187.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.271E-03	8.000E-01	20	B200	1 0 0 0 2	
4.271E-03	8.000E-01	21	M161	1 0 0 0 2	
4.698E-03	8.800E-01	22	K137	1 1 2 1 0	
4.698E-03	8.800E-01	25	P434	0 0 0 0 0	
<5.33E-03	<9.99E-01	ns	B185	0 0 0 0 0	
4.869E-03	9.120E-01	ns	F019	0 0 0 0 2	
5.334E-03	9.990E-01	ns	M061	0 0 0 0 0	

1901. $C_9H_{17}NO_3$
Diethylaceturethane
Detonal
RN: **MP** (°C)**:**
MW: 187.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.796E-02	5.236E+00	ns	O021	0 2 0 0 0	

1902. $C_9H_{17}NO_4$
3,3-Dihydroxy-2,2,5,5-tetramethyl-4-carbamyltetrahydrofuran
3-Furamide, tetrahydro-4,4-dihydroxy-2,2,5,5-tetramethyl-
RN: 29839-68-7 **MP** (°C)**:**
MW: 203.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.473E-01	9.091E+01	rt	B066	0 2 0 0 1	

1903. $C_9H_{17}N_5O$
Atratone
2-Methoxy-4-ethylamino-6-isopropylamino-*s*-triazine
2-Methoxy-4-ethylamino-6-isopropylamino-*s*-triazines
RN: 1610-17-9 **MP** (°C)**:**
MW: 211.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.520E-03	1.800E+00	20	B185	0 0 0 0 0	
8.520E-03	1.800E+00	20	M061	1 0 0 0 2	
8.520E-03	1.800E+00	21	B192	0 0 0 0 2	
8.520E-03	1.800E+00	21	G099	2 0 0 1 0	
7.905E-03	1.670E+00	25	H073	2 1 1 2 2	
1.240E-02	2.620E+00	50	G001	1 0 1 1 2	
9.448E-03	1.996E+00	ns	B100	0 0 0 0 0	
8.520E-03	1.800E+00	ns	C101	0 0 0 0 1	
7.829E-03	1.654E+00	ns	J033	0 0 0 0 0	

1904. $C_9H_{17}N_5S$

Ametryn
(2-Methylthio-4-ethylamino-6-isopropylamino-*s*-triazine
Ametryne
N-Ethyl-*N′*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine
Ametrex

RN: 834-12-8 **MP** (°C)**:** 84
MW: 227.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-04	1.841E-01	20	B200	1 0 0 0 1	
8.358E-04	1.900E-01	20	F311	1 2 2 2 1	
8.138E-04	1.850E-01	20	M161	1 0 0 0 2	
9.194E-04	2.090E-01	25	H073	2 1 1 2 2	
1.660E-03	3.774E-01	50	G001	1 0 1 1 2	
8.138E-04	1.850E-01	ns	C101	0 0 0 0 1	
8.490E-04	1.930E-01	ns	J033	0 0 0 0 0	

1905. C_9H_{18}

1-Nonene
α-Nonene
1-*n*-Nonene
n-Non-1-ene

RN: 124-11-8 **MP** (°C)**:** –81
MW: 126.24 **BP** (°C)**:** 146.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.850E-06	1.117E-03	25	M342	1 0 1 1 2	

1906. C_9H_{18}

1,1,3-Trimethylcyclohexane
Cyclogeraniolane

RN: 3073-66-3 **MP** (°C)**:** –65.7
MW: 126.24 **BP** (°C)**:** 136.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-05	1.770E-03	25	K119	1 0 0 0 2	
1.402E-05	1.770E-03	25	P051	2 1 1 2 2	
1.402E-05	1.770E-03	25.00	P007	2 1 2 2 2	

1907. $C_9H_{18}N_2O_2S$
Thiofanox
3,3-Dimethyl-1-(methylthio)-2-butanone *O*-((methylamino)carbonyl)oxime
Thiophanox
DS-15647
Dacamox
RN: 39196-18-4 **MP** (°C)**:** 57
MW: 218.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	5.200E+00	22	M161	1 0 0 0 1	

1908. $C_9H_{18}N_2O_4$
Meprobamate
2-Methyl-2-propyl-1,3-propanediol dicarbamate
Deprol
Meprospan
Miltown
Pathibamate
RN: 57-53-4 **MP** (°C)**:** 104
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.841E-02	6.200E+00	25	C039	1 2 2 1 1	form II
1.512E-02	3.300E+00	25	C039	1 2 2 1 1	form I
1.512E-02	3.300E+00	25	D082	1 0 1 0 1	
3.757E-02	8.200E+00	30	C039	1 2 2 1 1	form II
1.970E-02	4.300E+00	30	C039	1 2 2 1 1	form I
2.612E-02	5.700E+00	35	C039	1 2 2 1 1	form I
4.857E-02	1.060E+01	35	C039	1 2 2 1 2	form II
3.391E-02	7.400E+00	40	C039	1 2 2 1 1	form I
5.865E-02	1.280E+01	40	C039	1 2 2 1 2	form II

1909. $C_9H_{18}N_3S_6Fe$
Ferbam
tris(Dimethyldithiocarbamate)iron
Knockmate
Ferbeck
Hexaferb
Trifungol
RN: 14484-64-1 **MP** (°C)**:**
MW: 416.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.881E-04	1.200E-01	rt	I314	0 0 0 0 0	
3.121E-04	1.300E-01	rt	M161	0 0 0 0 2	

1910. $C_9H_{18}N_6$
Altretamine
Hexamethylmelamine
2,4,6-tris(Dimethylamino)-1,3,5-triazine
HMM
Hexastat
Hemel
RN: 645-05-6 **MP** (°C)**:** 172.0
MW: 210.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.846E-04	8.088E-02	25	B386	0 0 0 0 0	
4.327E-04	9.100E-02	25	C051	1 2 1 1 1	pH 7
4.150E-04	8.727E-02	25	K043	2 0 0 0 0	extrapolated

1911. $C_9H_{18}N_6$
1,3,5-Triazine-2,4,6-triamine, *N,N′,N″*-Triethyl-
*N*2,*N*4,*N*6-Triethylmelamine
tris(Ethylamino)-1,3,5-triazine
2,4,6-tris(Ethylamino)-1,3,5-triazine
2,4,6-tris(Ethylamino)-*s*-triazine
N,N′,N″-Triethyl-1,3,5-triazine-2,4,6-triamine
RN: 16268-92-1 **MP** (°C)**:**
MW: 210.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.318E-03	1.539E+00	25	B386	0 0 0 0 0	

1912. $C_9H_{18}N_6O$
N-Methylolpentamethylmelamine
N-(Hydroxymethyl)pentamethylmelamine
(Hydroxymethyl)pentamethylmelamine
RN: 16269-01-5 **MP** (°C)**:** 121.0
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.977E-03	9.000E-01	25	C051	1 2 1 1 0	pH 7, unstable in water

1913. $C_9H_{18}N_6O$
Ethanol, 2-[[4,6-bis(dimethylamino)-*s*-triazin-2-yl]amino]-
Ethanol, 2-[[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]amino]-
RN: 31482-09-4 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-02	2.562E+00	25	B386	0 0 0 0 0	

1914. $C_9H_{18}N_6O_3$
*N*2,*N*4,*N*6-Trimethyl-*N*2,*N*4,*N*6-trimethylolmelamine
N,N′,N″-Trimethyl-*N,N′,N″*-trimethylolmelamine
Trimelamol
CB 10-375
RN: 64124-21-6 **MP** (°C)**:** 129
MW: 258.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	9.040E+00	25	C051	1 2 1 1 2	pH 7

1915. $C_9H_{18}O$
Nonyl aldehyde
n-Nonanal
RN: 124-19-6 **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:** 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.749E-04	9.600E-02	25	A049	1 0 0 0 1	

1916. $C_9H_{18}O$
5-Nonanone
Dibutyl ketone
RN: 502-56-7 **MP** (°C)**:** –50
MW: 142.24 **BP** (°C)**:** 186.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.078E-01	10	G032	1 2 1 1 2	
1.800E-03	2.560E-01	25	K012	1 0 0 0 1	
2.550E-03	3.627E-01	30	G032	1 2 1 1 2	
2.430E-03	3.457E-01	50	G032	1 2 1 1 2	

1917. $C_9H_{18}O$
3-Hydroxy-2,3,4,5,5-pentamethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-01	9.091E+01	rt	B066	0 2 0 0 1	

1918. $C_9H_{18}O$

2,6-Dimethyl-4-heptanone
Diisobutyl ketone
RN: 108-83-8 **MP** (°C)**:**
MW: 142.24 **BP** (°C)**:** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	2.633E+00	23.50	O005	2 0 2 2 2	

1919. $C_9H_{18}O$

2-Nonanone
Nonan-2-one
RN: 821-55-6 **MP** (°C)**:** –21
MW: 142.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-03	1.900E-01	25	L450	0 0 0 0 0	

1920. $C_9H_{18}O_2$

3-Hydroxy-2-isopropyl-5,5-dimethyltetrahydrofuran
3-Furanol, tetrahydro-2-isopropyl-5,5-dimethyl-
RN: 29839-66-5 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.009E-01	4.762E+01	rt	B066	0 2 0 0 0	

1921. $C_9H_{18}O_2$

Pelargonic acid
1-Octanecarboxylic acid
Nonylic acid
n-Nonanoic acid
RN: 112-05-0 **MP** (°C)**:** 12
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.847E-04	1.400E-01	0	B136	1 0 2 1 1	
1.795E-03	2.840E-01	20	B136	1 0 2 1 2	
1.643E-03	2.599E-01	20.0	R001	1 1 1 1 1	
2.003E-03	3.170E-01	30	B136	1 0 2 1 2	
1.340E-03	2.120E-01	30	E005	2 1 1 2 2	
2.022E-03	3.199E-01	30.0	R001	1 1 1 1 1	
2.496E-03	3.950E-01	40	B136	1 0 2 1 2	
1.403E-03	2.220E-01	40	E005	2 1 1 2 2	
2.591E-03	4.100E-01	45	B136	1 0 2 1 1	
2.590E-03	4.098E-01	45.0	R001	1 1 1 1 1	

(*continued*)

1921. $C_9H_{18}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-03	2.640E-01	50	E005	2 1 1 2 2	
3.223E-03	5.100E-01	60	B136	1 0 2 1 1	
1.890E-03	2.990E-01	60	E005	2 1 1 2 2	
3.221E-03	5.097E-01	60.0	R001	1 1 1 1 1	
8.846E-04	1.400E-01	.0	R001	1 1 1 1 1	

1922. $C_9H_{18}O_2$
Methyl octanoate
Methyl caprylate
Methyl octylate
RN: 111-11-5 **MP** (°C)**:** –37
MW: 158.24 **BP** (°C)**:** 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.069E-04	6.440E-02	20	M337	2 1 2 2 2	

1923. $C_9H_{18}O_2$
3-Hydroxy-5-propyl-2,5-dimethyltetrahydrofuran
3-Furanol, 2,5-dimethyltetrahydro-5-propyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-01	2.913E+01	rt	B066	0 2 0 0 0	

1924. $C_9H_{18}O_2$
3-Hydroxy-5-methyl-5-isobutyltetrahydrofuran
3-Furanol, 5-isobutyltetrahydro-5-methyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1925. $C_9H_{18}O_2$
3-Hydroxy-5-methyl-5-butyltetrahydrofuran
3-Furanol, 5-butyltetrahydro-5-methyl-
RN: **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.518E-02	3.984E+00	rt	B066	0 2 0 0 0	

1926. $C_9H_{18}O_2$
3-Hydroxy-3-ethyl-2,2,5-trimethyltetrahydrofuranol
3-Furanol, 3-ethyltetrahydro-2,2,5-trimethyl-
RN: 29839-58-5 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.134E-01	6.542E+01	rt	B066	0 2 0 0 0	

1927. $C_9H_{18}O_2$
3-Hydroxy-2-methyl-2,5-diethyltetrahydrofuran
3-Furanol, 2,5-diethyltetrahydro-2-methyl-
RN: 29839-64-3 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	1.961E+01	rt	B066	0 2 0 0 0	

1928. $C_9H_{18}O_2$
3-Hydroxy-2,2,4,5,5-pentamethyltetrahydrofuran
3-Furanol, tetrahydro-2,2,4,5,5-pentamethyl-
RN: 29839-76-7 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1929. $C_9H_{18}O_2$
Butyl valerate
n-Butyl pentanoate
Butyl valerianate
RN: 591-68-4 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:** 186–187

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	8.387E-02	25	K012	1 0 0 0 1	

1930. $C_9H_{18}O_2$
Pentyl butyrate
n-Amyl *n*-butyrate
Pentyl *n*-butanoate
RN: 540-18-1 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	1.741E-01	20	S006	1 0 0 0 1	

1931. $C_9H_{18}O_2$
3-Hydroxy-2-methyl-5,5-diethyltetrahydrofuran
3-Furanol, 5,5-diethyltetrahydro-2-methyl-
RN: 6744-54-3 **MP** (°C)**:**
MW: 158.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.144E-02	4.975E+00	rt	B066	0 2 0 0 0	

1932. $C_9H_{18}O_3$
2,2-Diethyl-5-methyl-tetrahydrofuran-3,4-diol
3,4-Furandiol, 2,2-diethyltetrahydro-5-methyl-
RN: 31889-35-7 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.565E-01	1.667E+02	rt	B066	0 2 0 0 1	

1933. $C_9H_{18}O_3$
n-Propyl β-*n*-propoxypropionate
Propanoic acid, 3-propoxy-, propyl ester
RN: 14144-41-3 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-02	3.587E+00	25	R034	0 0 0 0 1	

1934. $C_9H_{18}O_3$
n-Amyl β-methoxypropionate
Pentyl 3-methoxypropionate
RN: 10500-16-0 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-02	2.892E+00	25	R034	0 0 0 0 1	

1935. $C_9H_{18}O_3$
1,3-Dioxolane-4-methanol, 2-butyl-2-methyl
RN: 5694-76-8 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.380E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

1936. $C_9H_{18}O_3$
n-Butyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, butyl ester
RN: 14144-35-5 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.287E-02	3.984E+00	25	D002	1 2 1 1 1	

1937. $C_9H_{18}O_3$
Hexyl lactate
Propanoic acid, 2-hydroxy-, hexyl ester
RN: 20279-51-0 **MP** (°C)**:**
MW: 174.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.700E+00	25	R006	2 2 0 1 1	

1938. $C_9H_{19}NOS$
Eptam
EPTC
Ethyl *N,N′*-di-*n*-propylthiolcarbamate
S-Ethyl dipropylthiocarbamate
S-Ethyl *N,N*-di-*n*-propylthiocarbamate
RN: 759-94-4 **MP** (°C)**:** <25
MW: 189.32 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-03	6.360E-01	3	G319	0 0 0 0 0	
1.954E-03	3.700E-01	20	B200	1 0 0 0 2	
1.981E+01	3.750E+03	20	F019	1 0 0 0 2	*sic*
1.981E-03	3.750E-01	20	M061	1 0 0 0 2	
1.928E-03	3.650E-01	20	M161	1 0 0 0 2	
4.170E+00	7.895E+02	25	B185	0 0 0 0 0	*sic*
1.981E-03	3.750E-01	25	G319	0 0 0 0 0	
1.981E-03	3.750E-01	25	M131	0 0 0 0 2	
2.123E-03	4.020E-01	28	H109	1 0 0 0 2	
1.981E-03	3.750E-01	ns	V414	0 0 0 0 0	

1939. $C_9H_{19}NO_2$
n-Octyl carbamate
Carbamic acid, octyl ester
RN: 2029-64-3 **MP** (°C)**:** 67
MW: 173.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	8.663E-02	37	H006	1 2 2 1 0	

1940. $C_9H_{19}O_3$
3-Hydroxy-4-methylol-2,2,5,5-tetramethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 175.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.119E-01	1.961E+01	rt	B066	0 2 0 0 0	

1941. C_9H_{20}
3,3-Diethylpentane
Tetraethylmethane
RN: 1067-20-5 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-06	1.212E-03	25	D346	0 0 0 0 0	

1942. C_9H_{20}
2,5-Dimethylheptane
RN: 2216-30-0 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1943. C_9H_{20}
3-Methyloctane
Octane, 3-methyl-
RN: 2216-33-3 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.237E-06	8.000E-04	23	C332	0 0 0 0 0	

1944. C_9H_{20}
2-Methyl-4-ethylhexane
RN: 3074-75-7 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E-06	3.590E-04	ns	S460	0 0 0 0 0	

1945. C_9H_{20}
2,2,3-Trimethylhexane
RN: 16747-25-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-06	3.623E-04	ns	S460	0 0 0 0 0	

1946. C_9H_{20}
2,4-Dimethylheptane
RN: 2213-23-2 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 133

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.938E-06	3.768E-04	ns	S460	0 0 0 0 0	

1947. C_9H_{20}
2,2,5-Trimethylhexane
Hexane, 2,2,5-trimethyl-
RN: 3522-94-9 **MP** (°C)**:** –120
MW: 128.26 **BP** (°C)**:** 124.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.159E-06	7.900E-04	0	P003	2 2 2 2 1	
8.966E-06	1.150E-03	25	M001	2 1 2 2 2	
4.210E-06	5.400E-04	25	P003	2 2 2 2 1	

1948. C_9H_{20}
2,2-Dimethylheptane
RN: 1071-26-7 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	3.592E-04	ns	S460	0 0 0 0 0	

1949. C_9H_{20}
Nonane
n-Nonan
RN: 111-84-2 **MP** (°C)**:** –53
MW: 128.26 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.72E-05	<2.20E-03	20	M337	2 1 2 2 1	
9.512E-07	1.220E-04	25	K119	1 0 0 0 2	
1.715E-06	2.200E-04	25	M003	1 0 2 2 2	
1.333E-06	1.710E-04	25	T423	0 0 0 0 0	
9.512E-07	1.220E-04	25.0	P051	2 1 1 2 2	
9.512E-07	1.220E-04	25.00	P007	2 1 2 2 2	
2.409E-06	3.090E-04	69.7	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.1	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.10	P007	2 1 2 2 2	
1.325E-05	1.700E-03	121.3	P051	2 1 1 2 2	
1.325E-05	1.700E-03	121.30	P007	2 1 2 2 2	
3.953E-05	5.070E-03	136.6	P051	2 1 1 2 2	
3.953E-05	5.070E-03	136.60	P007	2 1 2 2 2	

1950. C_9H_{20}
4,4-Dimethylheptane
RN: 1068-19-5 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-06	3.335E-04	ns	S460	0 0 0 0 0	

1951. C_9H_{20}
2,6-Dimethylheptane
RN: 1072-05-5 **MP** (°C)**:** –103
MW: 128.26 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.594E-06	3.327E-04	ns	S460	0 0 0 0 0	

1952. C_9H_{20}
3,5-Dimethylheptane
RN: 926-82-9 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1953. C_9H_{20}
3-Ethylheptane
RN: 15869-80-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.714E-06	2.198E-04	ns	S460	0 0 0 0 0	

1954. C_9H_{20}
4-Ethylheptane
RN: 2216-32-2 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-06	2.422E-04	ns	S460	0 0 0 0 0	

1955. C_9H_{20}
2,3-Dimethylheptane
RN: 3074-71-3 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.959E-06	2.512E-04	ns	S420	0 0 0 0 0	

1956. C_9H_{20}
2,3,4-Trimethylhexane
RN: 921-47-1 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.113E-06	2.711E-04	ns	S460	0 0 0 0 0	

1957. C_9H_{20}
3-Ethyl-2-methylhexane
2-Methyl-3-ethylhexane
RN: 16789-46-1 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E-06	2.871E-04	ns	S460	0 0 0 0 0	

1958. C_9H_{20}
3,3-Dimethylheptane
RN: 4032-86-4 **MP** (°C)**:**
MW: 128.26 **BP** (°C)**:** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-06	3.028E-04	ns	S460	0 0 0 0 0	

1959. C_9H_{20}
4-Methyloctane
4-Metylooktan
RN: 2216-34-4 **MP** (°C)**:** –113
MW: 128.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.966E-07	1.150E-04	25	K119	1 0 0 0 2	
8.966E-07	1.150E-04	25	P051	2 1 1 2 2	
8.966E-07	1.150E-04	25.00	P007	2 1 2 2 2	

1960. $C_9H_{20}NO_3PS_2$
Fostion
FAC 20
O,O-Diethyl *S*-(*N*-isopropylcarbamylmethyl) dithiophosphate
Prothoate
RN: 2275-18-5 **MP** (°C)**:** 24.5
MW: 285.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.761E-03	2.500E+00	20	M161	1 0 0 0 1	

1961. $C_9H_{20}O$
2,6-Dimethyl-4-heptanol
Diisobutylcarbinol
RN: 108-82-7 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.925E-03	9.990E-01	25	C093	2 1 1 1 1	

1962. $C_9H_{20}O$
n-Nonyl alcohol
Nonanol
RN: 143-08-8 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.340E-04	1.347E-01	20	H330	0 0 0 0 0	
9.700E-04	1.399E-01	25	K025	2 2 1 1 2	

1963. $C_9H_{20}O$
3-Ethyl-3-heptanol
RN: 19780-41-7 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	5.485E-01	ns	S460	0 0 0 0 0	

1964. $C_9H_{20}O$
2,6-Dimethyl-3-heptanol
RN: 19549-73-6 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.097E-03	4.468E-01	ns	S460	0 0 0 0 0	

1965. $C_9H_{20}O$
3-Nonanol
Hexyl ethyl carbinol
Ethyl *n*-hexyl carbinol
RN: 624-51-1 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.999E-03	2.884E-01	ns	J300	0 0 0 0 0	

1966. $C_9H_{20}O$

3,5,5-Trimethylhexanol
3.,5,5-Trimethyl hexanol
Nonylol
3,5,5-Trimethyl-1-hexanol
RN: 3452-97-9 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.501E-01	20	H330	0 0 0 0 0	
3.099E-03	4.470E-01	ns	J300	0 0 0 0 0	

1967. $C_9H_{20}O$

Methyl-octyl-alcohol
2-Nonanol
Heptylmethylcarbinol
Methyl *n*-heptyl carbinol
RN: 628-99-9 **MP** (°C)**:**
MW: 144.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.00E-03	<5.77E-01	25	F044	1 0 0 0 0	

1968. $C_9H_{21}N$

Tripropylamine
Tri-*n*-propylamine
N,N-Dipropylpropanamine
N,N-Dipropyl-1-propanamine
RN: 102-69-2 **MP** (°C)**:** –93.5
MW: 143.27 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E-03	7.473E-01	25.04	V013	2 2 2 2 2	

1969. $C_9H_{21}O_2PS_3$

Terbufos
O,O-Diethyl *S*-(((1,1-dimethylethyl)thio)methyl) phosphorodithoic acid
Counter 15G
Contraven
ST 100
RN: 13071-79-9 **MP** (°C)**:**
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-05	5.500E-03	19	B169	2 1 1 1 1	
1.758E-05	5.070E-03	24	F179	2 2 2 2 2	
1.907E-05	5.500E-03	ns	B325	0 1 0 0 1	

(*continued*)

1969. $C_9H_{21}O_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	1.000E-02	ns	M110	0 0 0 0 0	EFG
4.334E-05	1.250E-02	ns	M161	0 0 0 0 0	

1970. $C_9H_{21}O_3P$
Dibutyl methyl phosphonate
Di-*n*-butyl methanephosphonate
RN: 2404-73-1 **MP** (°C)**:**
MW: 208.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.842E-02	8.000E+00	25	B070	1 2 0 1 0	

1971. $C_9H_{21}O_3PS_3$
S-Ethylsulphinylmethyl *O,O*-di-isopropyl phosphorodithioate
O,O-Diisopropyl *S*-[(ethylsulfinyl)methyl] dithiophosphate
Aphidan
PSP 204
IPSP
RN: 5827-05-4 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E-03	1.500E+00	15	M161	1 0 0 0 1	

1972. $C_9H_{21}O_3PS_3$
Terbufos sulfoxide
Phosphorodithioic acid, *S*-[[(1,1-dimethylethyl)sulfinyl]methyl] *O,O*-diethyl ester
RN: 10548-10-4 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.61E-03	>1.10E+00	ns	B325	0 1 0 0 1	

1973. $C_9H_{21}O_4P$
Tripropyl phosphate
Tri-*n*-propyl phosphate
RN: 513-08-6 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	6.951E+00	30	V300	2 2 0 1 0	

1974. $C_9H_{21}O_4P$
Dibutyl methyl phosphate
Methyl dibutyl phosphate
RN: 7242-59-3 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.166E-02	7.100E+00	25	B070	1 2 2 1 1	

1975. $C_9H_{21}O_4P$
Diethyl amyl phosphate
O,O-Diethyl *O*-pentyl phosphate
Diethyl pentyl phosphate
RN: 20195-08-8 **MP** (°C)**:**
MW: 224.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.345E-02	7.500E+00	25	B070	1 2 0 1 1	

1976. $C_9H_{21}O_4PS_3$
Terbufos sulfone
Phosphorodithioic acid, *S*-[[(1,1-dimethylethyl)sulfonyl]methyl] *O,O*-diethyl ester
Counter sulfone
AC 94320
RN: 56070-16-7 **MP** (°C)**:**
MW: 320.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-03	4.078E-01	18.50	B169	2 0 1 1 2	
1.273E-03	4.078E-01	ns	B325	0 1 0 0 1	

1977. $C_9H_{22}O_4P_2S_4$
Ethion
O,O,O,O-Tetraethyl *S,S*-methylene bisphosphorodithioate
Nialate
Ethanox
Diethion
Hylemox
RN: 563-12-2 **MP** (°C)**:** –25
MW: 384.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-06	5.700E-04	10	B324	0 0 0 0 0	
1.483E-06	5.702E-04	10	B324	0 0 0 0 0	
2.861E-06	1.100E-03	19.50	B169	2 2 1 1 1	
1.769E-06	6.801E-04	20	B324	0 0 0 0 0	
1.769E-06	6.800E-04	20	B324	0 0 0 0 0	

(*continued*)

1977. $C_9H_{22}O_4P_2S_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-06	7.601E-04	30	B324	0 0 0 0 0	
1.977E-06	7.600E-04	30	B324	0 0 0 0 0	

1978. $C_{10}H_4Cl_2O_2$

Dichlone
2,3-Dichloro-1,4-naphthalenedione
Phygon XL
Phygon
Phygon paste
USR 604

RN: 117-80-6 **MP** (°C)**:**
MW: 227.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.404E-07	1.000E-04	25	M161	1 0 0 0 0	
3.083E-05	7.000E-03	ns	B160	0 0 0 0 0	
4.404E-06	1.000E-03	ns	B185	0 0 0 0 0	

1979. $C_{10}H_5ClN_2O_4$

1-Chloro-2,4-dinitronaphthalene
2,4-Dinitro-1-naphthyl chloride
2,4-Dinitrochloronaphthalene
2,4-Dinitro-1-chloronaphthalene

RN: 2401-85-6 **MP** (°C)**:** 148
MW: 252.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-06	1.000E-03	25	M061	1 0 0 0 0	

1980. $C_{10}H_5Cl_7$

Heptachlor
1,4,5,6,7,8,8-Heptachloro-3α,4,7,7α-tetrahydro-4,7-methano-1H-indene
3-Chlorochlordene
Tetrahydro
Rhodiachlor
3,4,5,6,7,8,8α-Heptachlorodicyclopentadiene

RN: 76-44-8 **MP** (°C)**:** 95.5
MW: 373.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-07	1.000E-04	15	B083	2 2 1 2 2	particle size 5 µm
4.786E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.822E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 µm

(*continued*)

1980. $C_{10}H_5Cl_7$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-07	5.600E-05	25	I308	0 0 0 0 0	
1.500E-07	5.600E-05	26.5	P027	1 1 2 2 1	
1.500E-07	5.600E-05	27	M161	0 0 0 0 1	
8.438E-07	3.150E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.313E-06	4.900E-04	45	B083	2 2 1 2 2	particle size 5 µm
8.036E-08	3.000E-05	ns	K138	0 0 0 0 2	
1.875E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
4.822E-07	1.800E-04	ns	V414	0 0 0 0 0	

1981. $C_{10}H_5Cl_7O$

Heptachlor epoxide
1,4,5,6,7,8,8-Heptachloro-2,3-epoxy-3α,4,7,7α-tetrahydro-4,7-methanoindan
Hepachlor epoxide

RN: 1024-57-3 **MP** (°C)**:** 160
MW: 389.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-07	1.100E-04	15	B083	2 2 1 2 2	particle size 5 µm
5.137E-07	2.000E-04	25	B083	2 2 1 2 2	particle size 5 µm
5.137E-07	2.000E-04	25	I308	0 0 0 0 0	
8.990E-07	3.500E-04	25	W025	1 0 2 2 2	
8.990E-07	3.500E-04	26.5	P027	1 1 2 2 1	
8.990E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.541E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.798E-06	7.000E-04	ns	M110	0 0 0 0 0	EFG
5.137E-07	2.000E-04	ns	V414	0 0 0 0 0	

1982. $C_{10}H_5N_3O_6$

1,3,8-Trinitronaphthalene
1,3,8-Trinitronaphthalin

RN: 2364-46-7 **MP** (°C)**:**
MW: 263.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-05	1.800E-02	15	F300	1 0 0 0 1	

1983. $C_{10}H_5N_3O_6$

1,4,5-Trinitronaphthalene
1,4,5-Trinitronaphthalin

RN: 2243-95-0 **MP** (°C)**:**
MW: 263.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.520E-04	4.000E-02	15	F300	1 0 0 0 1	

1984. $C_{10}H_6Br_2$
2,3-Dibromonaphthalene
Naphthalene, 2,3-dibromo-
RN: 13214-70-5 **MP** (°C)**:**
MW: 285.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-07	5.497E-05	4	D351	1 2 1 1 2	
4.778E-07	1.366E-04	25	D351	1 2 1 1 2	
1.222E-06	3.495E-04	40	D351	1 2 1 1 2	

1985. $C_{10}H_6Br_2$
1,4-Dibromonaphthalene
Naphthalene, 1,4-dibromo-
RN: 83-53-4 **MP** (°C)**:** 80–82
MW: 285.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.333E-07	1.239E-04	4	D351	1 2 1 1 2	
1.217E-06	3.479E-04	25	D351	1 2 1 1 2	
3.006E-06	8.595E-04	40	D351	1 2 1 1 2	

1986. $C_{10}H_6Cl_2$
1,4-Dichloronaphthalene
Naphthalene, 1,4-dichloro-
RN: 1825-31-6 **MP** (°C)**:**
MW: 197.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-06	2.628E-04	4	D351	1 2 1 1 2	
4.389E-06	8.649E-04	25	D351	1 2 1 1 2	
1.122E-05	2.212E-03	40	D351	1 2 1 1 2	

1987. $C_{10}H_6Cl_4O_3S$
Glenbar
O,S-Dimethyl tetrachlorothioterephthalate
RN: 3765-57-9 **MP** (°C)**:** 161
MW: 348.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.437E-06	5.000E-04	22	B200	1 0 0 0 0	
1.034E-06	3.600E-04	ns	M061	0 0 0 0 1	

1988. $C_{10}H_6Cl_4O_4$
Dimethyl tetrachloroterephthalate
DCPA
RN: 1861-32-1 **MP** (°C)**:** 156
MW: 331.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-06	5.000E-04	25	B200	1 0 0 0 0	
<1.51E-06	<5.00E-04	25	M161	1 0 0 0 0	
<1.51E-06	<5.00E-04	ns	B185	0 0 0 0 0	
1.506E-06	5.000E-04	ns	V414	0 0 0 0 0	

1989. $C_{10}H_6Cl_6$
Chlordene
4,5,6,7,8,8-Hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
RN: 3734-48-3 **MP** (°C)**:** –62
MW: 338.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.281E-06	7.730E-04	26.70	L071	1 2 0 1 2	

1990. $C_{10}H_6Cl_6O$
1-Hydroxychlordene
1-Hydroxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetra-hydro-4,7-methanoindene
RN: 2597-11-7 **MP** (°C)**:** 194
MW: 354.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.469E-06	1.231E-03	26.70	L071	1 2 0 1 2	

1991. $C_{10}H_6Cl_6O$
Chlordene epoxide
2,3-Epoxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
Chlordene hydroxide
4,7-Methano-1H-inden-1-ol, 4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-
RN: 6058-23-7 **MP** (°C)**:** 215
MW: 354.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.829E-06	1.359E-03	26.70	L071	1 2 0 1 2	

1992. $C_{10}H_6Cl_6O_2$
1-Hydroxychlordene epoxide
1-Hydroxy-2,3-epoxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene
RN: 24009-06-1 **MP** (°C)**:**
MW: 370.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.391E-06	2.741E-03	26.70	L071	1 1 1 1 2	

1993. $C_{10}H_6Cl_8$
cis-Chlordane
(1α,2α,3aα,4β,7β,7aα)-1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1α,2α,3aα,4β,7β,7aα)
α-Chlordane
RN: 5103-71-9 **MP** (°C)**:**
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1994. $C_{10}H_6Cl_8$
trans-Chlordane
(1α,2β,3aα,4β,7β,7aα)-1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-, (1α,2β,3aα,4β,7β,7aα)-
β-Chlordane
RN: 5103-74-2 **MP** (°C)**:**
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1995. $C_{10}H_6Cl_8$
Chlordane
1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3α,4,7,7α-tetrahydroindane
Octachlor
Velsicol 1068
Toxichlor
Ortho-Klor
RN: 57-74-9 **MP** (°C)**:** 105
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-07	5.657E-05	24.99	K436	0 0 0 0 0	
4.515E-06	1.850E-03	25	W025	1 0 2 2 2	
1.367E-07	5.600E-05	ns	K138	0 0 0 0 2	

(*continued*)

1995. $C_{10}H_6Cl_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
1.367E-07	5.600E-05	ns	S187	0 2 2 1 1	
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1996. $C_{10}H_6FN_3O_3$
3-Nicotinoyl-5-fluorouracil
RN: **MP** (°C)**:**
MW: 235.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E-02	2.700E+00	22	B332	1 1 0 0 1	pH 4.0

1997. $C_{10}H_6N_2O_4$
1,8-Dinitronaphthalene
1,8-Dinitronaphthalin
RN: 602-38-0 **MP** (°C)**:** 107
MW: 218.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-04	3.400E-02	15	F300	1 0 0 0 1	

1998. $C_{10}H_6N_2O_4$
1,5-Dinitronaphthalene
1,5-Dinitronaphthalin
RN: 605-71-0 **MP** (°C)**:** 216.5
MW: 218.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.658E-04	5.800E-02	12	F300	1 0 0 0 1	

1999. $C_{10}H_6O_8$
Pyromellitic acid
1,2,4,5-Benzenetetracarboxylic acid
Benzol-tetracarbonsaeure-(1,2,4,5)
RN: 89-05-4 **MP** (°C)**:**
MW: 254.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-02	1.400E+01	16	F300	1 0 0 0 2	

2000. $C_{10}H_7Br$
1-Bromonaphthalene
Naphthalene, 1-bromo-
RN: 90-11-9 **MP** (°C)**:** 6.2
MW: 207.08 **BP** (°C)**:** 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.383E-05	9.077E-03	4	D351	1 2 1 1 2	
4.733E-05	9.802E-03	10	D351	1 2 1 1 2	
4.500E-05	9.318E-03	21	A057	2 1 2 2 1	
6.444E-05	1.334E-02	25	D351	1 2 1 1 2	
9.166E-05	1.898E-02	40	D351	1 2 1 1 2	
6.000E-05	1.242E-02	ns	L060	0 0 0 0 0	
9.120E-05	1.889E-02	ns	S460	0 0 0 0 0	

2001. $C_{10}H_7Br$
2-Bromonaphthalene
Naphthalene, 2-bromo-
RN: 580-13-2 **MP** (°C)**:** 53.5
MW: 207.08 **BP** (°C)**:** 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.831E-03	4	D351	1 2 1 1 2	
3.883E-05	8.041E-03	25	D351	1 2 1 1 2	
7.611E-05	1.576E-02	40	D351	1 2 1 1 2	
4.000E-05	8.283E-03	ns	L060	0 0 0 0 0	

2002. $C_{10}H_7Cl$
β-Chloronaphthalene
2-Chloronaphthalene
RN: 91-58-7 **MP** (°C)**:** 59.5
MW: 162.62 **BP** (°C)**:** 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-06	<1.00E-03	30	M311	1 1 2 2 0	
8.000E-05	1.301E-02	ns	L060	0 0 0 0 0	

2003. $C_{10}H_7Cl$
1-Chloronaphthalene
α-Chloronaphthalene
1-Naphthyl chloride
RN: 90-13-1 **MP** (°C)**:** –20
MW: 162.62 **BP** (°C)**:** 259.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.23E-04	<2.00E-02	ns	L060	0 0 0 0 2	
1.164E-04	1.893E-02	ns	S460	0 0 0 0 0	

2004. $C_{10}H_7I$
α-Iodonaphthalene
1-Iodonaphthalene
RN: 90-14-2 **MP** (°C)**:**
MW: 254.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.114E-03	ns	L060	0 0 0 0 1	average
2.818E-05	7.161E-03	ns	S460	0 0 0 0 0	

2005. $C_{10}H_7NO_2$
1-Nitronaphthalene
1-Nitro-naphthalin
RN: 86-57-7 **MP** (°C)**:** 59.5
MW: 173.17 **BP** (°C)**:** 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-04	5.000E-02	18	F300	1 0 0 0 1	

2006. $C_{10}H_7NO_3$
1-Nitro-2-naphthol
1-Nitro-naphthol-(2)
RN: 550-60-7 **MP** (°C)**:** 104
MW: 189.17 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-03	2.000E-01	20	F300	1 0 0 0 2	

2007. $C_{10}H_7NO_3$
Kynurenic acid
4-Hydroxy-chinolin-carbonsaeure-(2)
Kynurensaeure
RN: 492-27-3 **MP** (°C)**:** 282.5
MW: 189.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-02	8.920E+00	100	D041	1 0 0 0 0	
4.969E-03	9.400E-01	100	F300	1 0 0 0 1	

2008. $C_{10}H_7N_3O_3$
Orotic acid pyridine
RN: **MP** (°C)**:**
MW: 217.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.606E+01	16	N018	0 0 0 0 0	

2009. $C_{10}H_7N_3S$
Thiabendazole
2-(Thiazol-4-yl)benzimidazole
Mintezol
Apl-Luster
Mertect
Tecto
RN: 148-79-8 **MP** (°C)**:** 304.5
MW: 201.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-04	5.000E-02	25	M161	1 0 0 0 1	intrinsic

2010. $C_{10}H_8$
Naphthalene
Napthalene
Mothballs
Camphor tar
RN: 91-20-3 **MP** (°C)**:** 80.2
MW: 128.18 **BP** (°C)**:** 217.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	1.730E-02	4.99	P331	0 0 0 0 0	
1.320E-04	1.692E-02	8.20	M082	1 1 1 2 2	
1.320E-04	1.692E-02	8.20	M151	2 1 2 2 1	
1.320E-04	1.692E-02	8.24	M183	1 2 1 1 2	
1.390E-04	1.782E-02	10	J302	2 1 2 2 2	
1.580E-04	2.025E-02	9.99	P331	0 0 0 0 0	
1.500E-04	1.923E-02	11.50	M082	1 1 1 2 2	
1.500E-04	1.923E-02	11.50	M151	2 1 2 2 2	
1.502E-04	1.925E-02	11.54	M183	1 2 1 1 2	
1.570E-04	2.012E-02	12	S076	2 2 2 2 2	
1.590E-04	2.038E-02	13.40	M082	1 1 1 2 2	
1.590E-04	2.038E-02	13.40	M151	2 1 2 2 2	
1.591E-04	2.039E-02	13.44	M183	1 2 1 1 2	
1.900E-04	2.435E-02	14.99	P331	0 0 0 0 0	
1.716E-03	2.200E-01	15	F300	1 0 0 0 2	*sic*
1.716E-04	2.200E-02	15	M073	1 0 2 2 1	
1.680E-04	2.153E-02	15.10	M082	1 1 1 2 2	

(*continued*)

2010. $C_{10}H_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-04	2.153E-02	15.10	M151	2 1 2 2 2	
1.677E-04	2.150E-02	15.14	M183	1 2 1 1 2	
1.900E-04	2.435E-02	18	S076	2 2 2 2 2	
2.010E-04	2.576E-02	19.30	M082	1 1 1 2 2	
2.010E-04	2.576E-02	19.30	M151	2 1 2 2 2	
2.013E-04	2.581E-02	19.34	M183	1 2 1 1 2	
2.240E-04	2.871E-02	19.99	P331	0 0 0 0 0	
1.748E-04	2.240E-02	20	A050	1 0 1 1 1	
7.412E-04	9.500E-02	20	B318	0 0 0 0 0	EFG
3.000E-04	3.845E-02	20	E009	1 0 0 0 1	
3.000E-04	3.845E-02	20	E025	1 0 2 2 1	
1.900E-04	2.435E-02	20	H306	1 0 1 2 1	
1.272E-04	1.630E-02	20	T301	1 2 2 2 2	
2.400E-04	3.076E-02	22	A413	2 0 2 2 1	
2.645E-04	3.390E-02	22	C413	2 0 2 2 1	
1.638E-04	2.100E-02	22	N311	1 0 1 1 2	
2.255E-04	2.890E-02	22.20	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	23	P332	0 0 0 0 0	
2.341E-04	3.000E-02	23	P339	0 0 0 0 0	
2.300E-04	2.948E-02	23.40	M082	1 1 1 2 2	
2.300E-04	2.948E-02	23.40	M151	2 1 2 2 2	
2.301E-04	2.949E-02	23.44	M183	1 2 1 1 2	
2.380E-04	3.050E-02	24.50	W003	2 2 2 2 2	average of 5
2.630E-04	3.371E-02	24.99	P331	0 0 0 0 0	
2.458E-04	3.150E-02	25	A001	1 2 2 2 2	
2.350E-04	3.012E-02	25	A325	2 1 2 2 2	
2.684E-04	3.440E-02	25	B003	2 2 2 2 2	
2.465E-04	3.160E-02	25	B319	2 0 1 2 2	average of 2
2.442E-04	3.130E-02	25	D337	0 0 0 0 0	
2.715E-04	3.480E-02	25	D406	1 2 2 2 2	
2.442E-04	3.130E-02	25	E004	2 1 2 2 2	
2.620E-04	3.358E-02	25	G047	2 2 2 2 2	
2.520E-04	3.230E-02	25	J302	2 1 2 2 2	
9.750E-05	1.250E-02	25	K001	2 2 2 2 2	
2.300E-04	2.948E-02	25	K123	1 0 2 2 1	
2.497E-04	3.200E-02	25	L332	1 1 1 1 0	
2.653E-04	3.400E-02	25	M040	1 0 0 1 1	
2.550E-04	3.268E-02	25	M058	2 2 2 2 2	
2.473E-04	3.170E-02	25	M064	1 1 2 2 2	
2.472E-04	3.169E-02	25	M071	2 2 2 2 2	
3.121E-04	4.000E-02	25	M073	1 0 2 2 1	
2.620E-04	3.358E-02	25	M123	1 0 0 0 2	
2.575E-04	3.300E-02	25	M130	1 0 0 0 1	
2.390E-04	3.063E-02	25	M342	1 0 1 1 2	
2.497E-04	3.200E-02	25	O320	0 0 0 0 0	
2.575E-05	3.300E-03	25	P340	0 0 0 0 0	
2.356E-04	3.020E-02	25	R042	1 2 2 2 2	

(*continued*)

2010. $C_{10}H_8$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-04	2.999E-02	25	S076	2 2 2 2 2	
1.716E-04	2.200E-02	25	S227	1 2 1 1 1	
2.390E-04	3.063E-02	25	W300	2 2 2 2 2	
2.490E-04	3.192E-02	25.00	M082	1 1 1 2 2	
2.490E-04	3.192E-02	25.00	M151	2 1 2 2 2	
2.472E-04	3.169E-02	25.00	M151	2 1 1 2 2	
6.936E-04	8.890E-02	25.00	P007	2 1 2 2 2	
2.492E-04	3.194E-02	25.04	M183	1 2 1 1 2	
2.510E-04	3.217E-02	25.04	V013	2 2 2 2 2	
2.660E-04	3.409E-02	27.00	M082	1 1 1 2 2	
2.660E-04	3.409E-02	27.00	M151	2 1 2 2 2	
2.666E-04	3.417E-02	27.04	M183	1 2 1 1 2	
2.980E-04	3.820E-02	29.90	W003	2 2 2 2 2	average of 3
3.240E-04	4.153E-02	29.99	P331	0 0 0 0 0	
2.949E-04	3.780E-02	30.30	W003	2 2 2 2 2	average of 3
3.448E-04	4.420E-02	34.50	W003	2 2 2 2 2	average of 2
3.710E-04	4.755E-02	34.99	P331	0 0 0 0 0	
4.112E-04	5.270E-02	39.30	W003	2 2 2 2 2	average of 2
4.360E-04	5.588E-02	39.99	P331	0 0 0 0 0	
4.275E-04	5.480E-02	40.10	W003	2 2 2 2 2	
5.118E-04	6.560E-02	44.70	W003	2 2 2 2 2	average of 3
6.132E-04	7.860E-02	50.20	W003	2 2 2 2 2	
8.270E-04	1.060E-01	55.60	W003	2 2 2 2 2	
1.233E-03	1.580E-01	64.50	W003	2 2 2 2 2	average of 3
1.904E-03	2.440E-01	73.40	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	ns	F071	0 1 2 1 1	
2.341E-04	3.000E-02	ns	H080	0 0 0 0 1	
2.473E-04	3.170E-02	ns	H123	0 0 0 0 0	
2.473E-04	3.170E-02	ns	K304	0 0 0 0 2	
2.340E-04	2.999E-02	ns	L060	0 0 0 0 2	average
2.473E-04	3.170E-02	ns	M344	0 0 0 0 2	
2.341E-04	3.000E-02	ns	O009	0 0 0 0 0	
8.129E-04	1.042E-01	ns	R042	1 2 2 2 2	
2.341E-04	3.000E-02	rt	M161	0 0 0 0 1	
2.848E-04	3.650E-02	rt	S314	0 0 2 1 2	

2011. $C_{10}H_8BrN_3O$

Bropirimine

2-Amino-5-bromo-6-phenyl-py-rimidin-4(3H)-one

ABPP

RN: 56741-95-8 **MP** (°C)**:**

MW: 266.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.931E-05	7.800E-03	37	A346	0 0 0 0 0	EFG

2012. $C_{10}H_8BrN_3O$
Brompyrazone
Amino-4-bromo-2-phenyl-3(2H)-pyridazinone
1-Phenyl-4-amino-5-bromo-6-pyridazone
Pyridazinone, 5-amino-4-bromo-2-phenyl-
RN: 3042-84-0 **MP** (°C)**:** 223.5
MW: 266.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.516E-04	2.000E-01	20	M161	1 0 0 0 2	

2013. $C_{10}H_8ClN_3O$
Pyrazon
5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone
RN: 1698-60-8 **MP** (°C)**:** 207
MW: 221.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.353E-03	3.000E-01	20	B185	0 0 0 0 0	
1.353E-03	2.999E-01	20	B200	1 0 0 0 0	
1.353E-03	2.999E-01	20	M061	1 0 0 0 0	
1.805E-03	4.000E-01	20	M161	1 0 0 0 2	

2014. $C_{10}H_8N_2$
γ,γ′-Dipyridyl
4,4′-Bipyridyl
RN: 553-26-4 **MP** (°C)**:** 69
MW: 156.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-02	4.509E+00	25	B095	2 0 1 1 2	

2015. $C_{10}H_8N_2$
α,α′-Dipyridyl
2,2′-Dipyridyl
α,α′-Bipyridyl
2,2′-Bipyridine
2,2′-Bipyridyl
RN: 366-18-7 **MP** (°C)**:** 71.5
MW: 156.19 **BP** (°C)**:** 273

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-02	5.000E+00	20	F300	1 0 0 0 0	
4.276E-02	6.678E+00	24.99	B444	0 0 0 0 0	
3.778E-02	5.900E+00	25	B095	2 0 1 1 2	
4.094E-02	6.394E+00	25	K063	2 2 0 1 2	

2016. $C_{10}H_8N_2O_2$
4-Phenyluracil
4-Phenyl-uracil
RN: 21321-07-3 **MP** (°C)**:**
MW: 188.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.314E-02	1.000E+01	100	F300	1 0 0 0 0	

2017. $C_{10}H_8O$
1-Naphthol
α-Naphthol
RN: 90-15-3 **MP** (°C)**:** 96
MW: 144.17 **BP** (°C)**:** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.030E-03	8.694E-01	11	K307	2 0 1 2 2	
7.700E-03	1.110E+00	20	K130	2 1 1 1 2	
7.700E-03	1.110E+00	20	K301	2 2 1 1 1	
7.700E-03	1.110E+00	20	K307	2 0 1 2 2	
6.001E-03	8.653E-01	24	H106	1 0 2 2 2	
6.007E-03	8.660E-01	24	M303	1 0 1 1 2	
3.029E-03	4.367E-01	25	L085	1 2 0 1 2	
9.430E-03	1.360E+00	30	K307	2 0 1 2 2	
1.490E-02	2.148E+00	40	K307	2 0 1 2 2	
2.150E-02	3.100E+00	50	K307	2 0 1 2 2	

2018. $C_{10}H_8O$
2-Naphthol
β-Naphthol
RN: 135-19-3 **MP** (°C)**:** 121
MW: 144.17 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	3.550E-01	6.90	M026	2 0 1 2 2	
3.378E-03	4.870E-01	13.45	M026	2 0 1 2 2	
3.473E-03	5.007E-01	15.60	M027	1 0 0 2 2	
3.646E-03	5.257E-01	16.20	M027	1 0 0 2 2	
3.891E-03	5.610E-01	17.70	M026	2 0 1 2 2	
4.450E-03	6.416E-01	20	K130	2 1 1 1 2	
4.500E-03	6.488E-01	20	K301	2 2 1 1 1	
4.450E-03	6.416E-01	20	K308	1 0 0 1 2	
5.800E-03	8.362E-01	20	M122	2 0 2 2 2	
4.945E-03	7.130E-01	21.50	M026	2 0 1 2 2	
4.713E-03	6.795E-01	23.20	M027	1 0 0 2 2	
3.954E-03	5.700E-01	25	F300	1 0 0 0 2	

(*continued*)

2018. $C_{10}H_8O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.240E-03	7.555E-01	25	K040	1 0 2 1 2	
5.356E-03	7.722E-01	25	L085	1 2 0 1 2	
6.929E-03	9.990E-01	25	R041	0 0 0 0 0	
6.076E-03	8.760E-01	29.50	M026	2 0 1 2 2	
6.431E-03	9.271E-01	31.30	M027	1 0 0 2 2	
6.832E-03	9.850E-01	33.30	M026	2 0 1 2 2	
9.045E-03	1.304E+00	38.70	M026	2 0 1 2 2	
1.116E-02	1.609E+00	44.50	M026	2 0 1 2 2	
1.388E-02	2.001E+00	49.50	M026	2 0 1 2 2	
1.706E-02	2.460E+00	55.20	M026	2 0 1 2 2	
2.104E-02	3.034E+00	60.00	M026	2 0 1 2 2	
2.928E-02	4.222E+00	68.10	M026	2 0 1 2 2	
3.810E-02	5.493E+00	75.00	M026	2 0 1 2 2	
4.670E-02	6.733E+00	80	K308	1 0 0 1 2	
5.129E-03	7.394E-01	ns	R427	0 0 0 0 0	

2019. $C_{10}H_8O_2$
2,3-Dihydroxynaphthalene
2,3-Dihydroxy-naphthalin
RN: 92-44-4 **MP** (°C)**:** 162
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-03	2.931E-01	20	M122	2 0 2 2 2	

2020. $C_{10}H_8O_2$
2,6-Dihydroxynaphthalene
2,6-Dihydroxy-naphthalin
RN: 581-43-1 **MP** (°C)**:**
MW: 160.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-03	1.000E+00	14	F300	1 0 0 0 0	

2021. $C_{10}H_9ClN_4O_2S$
2-Sulfanilamido-5-chloropyrimidine
Benzenesulfonamide, 4-amino-*N*-(5-chloro-2-pyrimidinyl)-
RN: 4482-46-6 **MP** (°C)**:**
MW: 284.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.322E-05	1.800E-02	37	R046	1 2 1 1 1	

2022. $C_{10}H_9ClN_4O_2S$
5-Sulfanilamido-2-chloropyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-chloro-5-pyrimidinyl)-
RN: 17103-49-0 **MP** (°C)**:**
MW: 284.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.127E-03	3.210E-01	37	R046	1 2 1 1 1	

2023. $C_{10}H_9Cl_2NO$
Acrylanilide, 3′,4′-dichloro-2-methyl-
Dicryl
RN: 2164-09-2 **MP** (°C)**:** 127–128
MW: 230.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-05	8.000E-03	ns	B185	0 0 0 0 0	

2024. $C_{10}H_9Cl_3O_3$
2,4,5-Trichlorophenoxy-γ-butyric acid
2,4,5-TB
4-(2,4,5-Trichlorophenoxy)butyric acid
4-(2,4,5-TB)
RN: 93-80-1 **MP** (°C)**:** 114.5
MW: 283.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-04	4.200E-02	25	B164	1 0 1 1 1	
1.481E-04	4.200E-02	ns	B185	0 0 0 0 0	

2025. $C_{10}H_9Cl_3O_3$
2,4-Dichlorophenoxyacetic acid β-monochloroethyl ester
Ethanol, 2-chloro-, (2,4-dichlorophenoxy)acetate
RN: 19810-30-1 **MP** (°C)**:**
MW: 283.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-04	5.415E-02	ns	M120	0 0 1 1 2	

2026. $C_{10}H_9Cl_4NO_2S$
Captafol
cis-3α,4,7,7α-Tetrahydro-2-(1,1,2,2-tetrachloroethyl)thio-1H-isoindole-1,3(2H)-dione
Crisfolatan
Difolatan
Folcid
RN: 2939-80-2 **MP** (°C)**:** 160.5
MW: 349.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-06	1.422E-03	20	B179	0 0 0 0 0	
4.011E-06	1.400E-03	ns	M161	0 0 0 0 1	

2027. $C_{10}H_9Cl_4O_4P$
Gardona
2-Chloro-1-(2,4,5-trichlorophenyl)vinyldimethylphosphate
RN: 22248-79-9 **MP** (°C)**:** 97.5
MW: 365.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M061	1 0 0 0 1	

2028. $C_{10}H_9Cl_4O_4P$
Tetrachlorvinphos
2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate
Rabon
Gardona
SD 8447
Stirofos
RN: 961-11-5 **MP** (°C)**:** 96
MW: 365.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M161	1 0 0 0 1	

2029. $C_{10}H_9N$
3-Methyl-isoquinoline
Isoquinoline, 3-methyl-
RN: 1125-80-0 **MP** (°C)**:**
MW: 143.19 **BP** (°C)**:** 519.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-03	9.190E-01	20	A050	1 0 1 1 2	

2030. $C_{10}H_9N$
2-Naphthylamine
Naphthylamine-(2)
β-Naphthylamin
β-Naphthylamine
RN: 91-59-8 **MP** (°C)**:** 113
MW: 143.19 **BP** (°C)**:** 306.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.320E-03	1.890E-01	rt	N015	0 0 2 2 2	

2031. $C_{10}H_9N$
1-Naphthylamine
1-Aminonaphthalene
α-Naphthoylamine
α-Naphthylamin
α-Naphthylamine
RN: 134-32-7 **MP** (°C)**:** 50
MW: 143.19 **BP** (°C)**:** 300.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	1.700E+00	20	F300	1 0 0 0 1	
3.600E-04	5.155E-02	ns	L060	0 0 0 0 1	average

2032. $C_{10}H_9NO$
8-Hydroxyquinaldine
2-Methyl 8-quinolinol
RN: 826-81-3 **MP** (°C)**:** 72.5
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E+03	3.916E+05	25.2	P024	2 2 1 1 2	
2.670E+03	4.250E+05	30.3	P024	2 2 1 1 2	

2033. $C_{10}H_9NO$
4-Hydroxy-2-methylquinoline
4-Hydroxy-2-methyl-chinolin
RN: 607-67-0 **MP** (°C)**:** 234
MW: 159.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.282E-02	1.000E+01	20	F300	1 0 0 0 1	
5.936E-01	9.450E+01	100	F300	1 0 0 0 2	

2034. $C_{10}H_9NO_2S$
Ethyl *m*-isothiocyanobenzoate
Ethyl 3-isothiocyanobenzoate
RN: 3137-84-6 **MP** (°C)**:**
MW: 207.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	5.181E-02	25	K032	2 2 0 1 2	

2035. $C_{10}H_9NO_2S$
Ethyl 4-isothiocyanatobenzoate
4-Carbethoxyphenylisothiocyanate
Ethyl *p*-isothiocyanatobenzoate
RN: 1205-06-7 **MP** (°C)**:**
MW: 207.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	1.865E-02	25	D019	1 1 1 1 1	

2036. $C_{10}H_9NO_3S$
Badische acid
2-Naphthylamine-8-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(8)
RN: 86-60-2 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-03	6.000E-01	20	F300	1 0 0 0 2	

2037. $C_{10}H_9NO_3S$
2-Naphthylamine-1-sulfonic acid
α-Naphthylamine-*o*-monosulfonic acid
RN: 81-16-3 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	2.394E+00	0	D077	1 0 0 1 1	
1.429E-02	3.190E+00	10	D077	1 0 0 1 1	
1.829E-02	4.083E+00	20	D077	1 0 0 1 1	
2.317E-02	5.173E+00	30	D077	1 0 0 1 1	
2.893E-02	6.458E+00	40	D077	1 0 0 1 1	
3.555E-02	7.937E+00	50	D077	1 0 0 1 1	
4.435E-02	9.901E+00	60	D077	1 0 0 1 2	
6.010E-02	1.342E+01	70	D077	1 0 0 1 2	
7.834E-02	1.749E+01	80	D077	1 0 0 1 2	
1.028E-01	2.296E+01	90	D077	1 0 0 1 2	
1.347E-01	3.007E+01	100	D077	1 0 0 1 2	

2038. $C_{10}H_9NO_3S$
1-Naphthylamine-8-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(8)
Peri acid
RN: 82-75-7 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	21	F300	1 0 0 0 0	
1.971E-02	4.400E+00	100	F300	1 0 0 0 1	

2039. $C_{10}H_9NO_3S$
1-Naphthylamine-5-sulfonic acid
Laurent's acid
Naphthylamin-(1)-sulfosaeure-(5)
RN: 84-89-9 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	20	F300	1 0 0 0 2	

2040. $C_{10}H_9NO_3S$
1-Naphthylamine-4-sulfonic acid
4-Amino-1-naphthalenesulfonic acid
Naphthionic acid
Naphthylamin-(1)-sulfosaeure-(4)
Pirias acid
RN: 84-86-6 **MP** (°C)**:** 000
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-03	2.699E-01	0	D077	1 0 0 1 1	
1.299E-03	2.899E-01	10	D077	1 0 0 1 1	
1.388E-03	3.099E-01	20	D077	1 0 0 1 1	
1.344E-03	3.000E-01	20	F300	1 0 0 0 0	
1.657E-03	3.699E-01	30	D077	1 0 0 1 1	
2.149E-03	4.798E-01	40	D077	1 0 0 1 1	
2.641E-03	5.897E-01	50	D077	1 0 0 1 1	
3.357E-03	7.494E-01	60	D077	1 0 0 1 1	
4.341E-03	9.691E-01	70	D077	1 0 0 1 1	
5.815E-03	1.298E+00	80	D077	1 0 0 1 2	
7.825E-03	1.747E+00	90	D077	1 0 0 1 2	
1.021E-03	2.279E-01	100	D077	1 0 0 1 2	
1.075E-02	2.400E+00	100	F300	1 0 0 0 1	

2041. $C_{10}H_9NO_3S$
1,6-Cleve's acid
1-Naphthylamine-6-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(6)
RN: 119-79-9 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	16	F300	1 0 0 0 2	

2042. $C_{10}H_9NO_3S$
Cassella's acid F
2-Naphthylamine-7-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(7)
RN: 494-44-0 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	20	F300	1 0 0 0 1	
1.389E-02	3.100E+00	100	F300	1 0 0 0 1	

2043. $C_{10}H_9NO_3S$
Bronner's acid
2-Naphthylamine-6-sulfonic acid
Naphthylamin-(2)-sulfosaeure-(6)
RN: 93-00-5 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.375E-04	1.200E-01	20	F300	1 0 0 0 1	
7.615E-03	1.700E+00	100	F300	1 0 0 0 1	

2044. $C_{10}H_9NO_3S$
1-Naphthylamine-2-sulfonic acid
Naphthylamin-(1)-sulfosaeure-(2)
RN: 81-06-1 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	4.100E+00	20	F300	1 0 0 0 1	
1.402E-01	3.130E+01	100	F300	1 0 0 0 2	

2045. $C_{10}H_9NO_3S$
2-Naphthylamine-5-sulfonic acid
Dahl's acid
Naphthylamin-(2)-sulfosaeure-(5)
RN: 81-05-0 **MP** (°C)**:**
MW: 223.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	3.300E-01	20	F300	1 0 0 0 2	

2046. $C_{10}H_9NO_4S$
7-Amino-1-naphthol-3-sulfonic acid
7-Amino-naphtol-(1)-sulfosaeure-(3)
RN: 90-51-7 **MP** (°C)**:**
MW: 239.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-02	4.500E+00	h	F300	0 0 0 0 1	

2047. $C_{10}H_9NO_9S_3$
1-Naphthylamine-2,4,7-trisulfonic acid
1,3,6-Naphthalenetrisulfonic acid, 4-amino-
RN: 61986-93-4 **MP** (°C)**:**
MW: 383.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.799E-01	1.840E+02	20	F054	1 2 1 1 2	
8.216E-01	3.150E+02	80	F054	1 2 1 1 2	

2048. $C_{10}H_9N_3O_3S$
1-Sulfanilyl-3-methyl-5-pyrazolone
RN: **MP** (°C)**:**
MW: 251.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-03	4.590E-01	37	R045	1 2 1 1 2	

2049. $C_{10}H_9N_4O_5$
Picrolonic acid
Pikrolonsaeure
RN: 550-74-3 **MP** (°C)**:** 116
MW: 265.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.394E-02	9.000E+00	17	F300	1 0 0 0 0	
3.582E-02	9.500E+00	100	F300	1 0 0 0 1	

2050. $C_{10}H_{10}Fe$
Ferrocene
bis-Cyclopentadienyliron
Ferrotsen
Iron bis(cyclopentadiene)
RN: 102-54-5 **MP** (°C)**:**
MW: 186.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-05	6.304E-03	25	B335	1 2 0 0 1	

2051. $C_{10}H_{10}BrNO_3S$
4-Thiazolidinecarboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-
RN: 256235-53-7 **MP** (°C)**:**
MW: 304.17 **BP** (°C)**:** 451.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.650E-01	21	B414	1 0 0 1 1	fast decomposition

2052. $C_{10}H_{10}BrNO_4$
5-Bromo-2-*p*-phenyl-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-5-nitro-2-phenyl-
1,3-Dioxane, 5-bromo-5-nitro-2-phenyl-
RN: 58522-87-5 **MP** (°C)**:** 82–84
MW: 288.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	4.598E-01	25	L013	1 0 2 1 2	

2053. $C_{10}H_{10}BrNO_5$
5-Bromo-2-*p*-phenol-5-nitro-1,3-dioxane
m-Dioxane, 5-bromo-5-nitro-2-phenol-
RN: 60766-61-2 **MP** (°C)**:** 142–144
MW: 304.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	4.298E-01	25	L013	1 0 2 1 2	

2054. $C_{10}H_{10}ClNO_2S$
4-Thiazolidinecarboxylic acid, 2-(4-chlorophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*p*-chlorophenyl)-
Thiazolidine-4-carboxylic acid, (2-(4-chlorophenyl)-
RN: 34491-29-7 **MP** (C)**:** 156-185 (°decomp)
MW: 243.71 **BP** (°C)**:** 458.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-03	1.438E+00	21	B414	1 0 0 1 1	fast decomposition

2055. $C_{10}H_{10}ClNO_2S$
4-Thiazolidinecarboxylic acid, 2-(2-chlorophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*o*-chlorophenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-chlorophenyl)-
RN: 72678-81-0 **MP** (°C)**:** 145–147
MW: 243.71 **BP** (°C)**:** 439.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.118E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2056. $C_{10}H_{10}ClNO_3$
Chloroacetyl acetaminophen
Acetic acid, chloro-, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, chloroacetate (ester)
RN: 17321-63-0 **MP** (°C)**:** 184.5–185
MW: 227.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	2.800E-01	37	D029	0 0 0 0 0	

2057. $C_{10}H_{10}Cl_2F_2N_2OS$
3-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-1,1-dimethylurea
N-[3-Chloro-4-(chlorodifluoromethylthiol)phenyl]-*N′,N′*-dimethylurea
N-(3-Chloro-4-difluorochloromethylthiophenyl)-*N′,N′*-dimethylurea
Thiochlormethyl
N-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-*N′,N′*-dimethylurea
RN: 33439-45-1 **MP** (°C)**:** 113.5
MW: 315.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.159E-01	6.803E+01	20	M161	1 0 0 0 1	

2058. $C_{10}H_{10}Cl_2O_2$
Chlorfenprop-methyl
Methyl 2-chloro-3-(*p*-chlorophenyl)propionate
Methyl α-*p*-dichlorohydrocinnamate
Bidisin
Fatex
RN: 14437-17-3 **MP** (°C)**:**
MW: 233.10 **BP** (°C)**:** 111.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.716E-04	4.000E-02	20	M161	1 0 0 0 1	

2059. $C_{10}H_{10}Cl_2O_3$
4-(2,4-Dichlorophenoxy)propionic acid
2,4-DB
RN: 94-82-6 **MP** (°C)**:** 118
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	6.700E-02	25	B164	1 0 1 1 1	
1.847E-04	4.600E-02	25	M161	1 0 0 0 1	
2.128E-04	5.300E-02	ns	B185	0 0 0 0 0	
1.847E-04	4.600E-02	ns	L024	1 0 0 0 1	
2.128E-04	5.300E-02	rt	M061	0 0 0 0 1	

2060. $C_{10}H_{10}Cl_2O_3$
Ethyl (2,4-dichlorophenoxy)acetate
2,4-Dichlorophenoxyacetic acid ethyl ester
RN: 533-23-3 **MP** (°C)**:**
MW: 249.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.529E-04	6.300E-02	ns	M120	0 0 1 1 2	

2061. $C_{10}H_{10}Cl_8$
Toxaphene
Camphechlor
Campheclor
PhenAcide
Toxakil
Chlorinated champhene
RN: 8001-35-2 **MP** (°C)**:** 65
MW: 413.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-06	5.500E-04	20	M336	2 0 2 2 2	
9.666E-07	4.000E-04	25	C100	1 0 2 1 0	
1.208E-06	5.000E-04	25	P085	0 0 0 0 0	
1.788E-06	7.400E-04	25	W025	1 0 2 2 2	
1.450E-06	6.000E-04	ns	M110	0 0 0 0 0	EFG
1.329E-06	5.500E-04	ns	V414	0 0 0 0 0	
7.250E-06	3.000E-03	rt	M161	0 0 0 0 0	

2062. $C_{10}H_{10}N_2O_4S$
4-Thiazolidinecarboxylic acid, 2-(3-nitrophenyl)-
4-Thiazolidinecarboxylic acid, 2-(*m*-nitrophenyl)-
RN: 69570-81-6 **MP** (°C)**:** 151–153
MW: 254.27 **BP** (°C)**:** 500.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.348E+00	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2063. $C_{10}H_{10}N_4O$
Metamitron
3-Methyl-4-amino-6-phenyl-1,2,4-triazin-5(4H)-one
4-Amino-3-methyl-6-phenyl-1,2,4-triazin-5-one
Goltix
RN: 41394-05-2 **MP** (°C)**:** 166.6
MW: 202.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.901E-03	1.800E+00	20	M161	1 0 0 0 1	

2064. $C_{10}H_{10}N_4O_2S$

Sulfadiazine
Sulphadiazine
*N*1-(2-Pyrimidinyl)-sulfanilamide
Debenal

RN: 68-35-9 **MP** (°C)**:** 254
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-04	5.907E-02	20	C006	1 2 1 1 2	
1.814E-04	4.540E-02	20	E003	2 2 1 1 2	
5.993E-04	1.500E-01	20	F073	1 2 2 2 2	
2.917E-04	7.299E-02	20	L058	1 0 1 1 1	
3.077E-04	7.700E-02	25	C102	2 0 2 2 2	
2.637E-03	6.600E-01	25	K048	1 2 2 1 1	pH 1.26
2.682E-04	6.713E-02	25	M440	0 0 0 0 0	
3.036E-04	7.599E-02	30	E003	2 2 1 1 2	
3.640E-04	9.110E-02	30	H018	0 0 0 0 0	
3.200E-04	8.009E-02	30	L069	1 0 1 1 0	EFG
7.192E-04	1.800E-01	35	H114	1 0 0 0 1	
5.074E-04	1.270E-01	37	C102	2 0 2 2 2	
4.914E-04	1.230E-01	37	F072	1 0 0 0 2	
4.794E-04	1.200E-01	37	F075	1 0 2 2 2	
5.114E-04	1.280E-01	37	K091	1 0 0 0 2	
5.194E-04	1.300E-01	37	L091	1 0 0 0 1	pH 5.5
7.192E-04	1.800E-01	37	M057	1 0 0 0 2	pH 5.5
8.790E-04	2.200E-01	37	R044	0 0 0 0 0	EFG, intrinsic
4.914E-04	1.230E-01	37	R045	1 2 1 1 1	
6.712E-04	1.680E-01	37	S192	1 0 1 1 2	pH 6.0
5.074E-04	1.270E-01	37	W016	2 0 1 1 2	
4.914E-04	1.230E-01	37	W053	1 0 0 0 2	
3.956E-04	9.900E-02	38	K006	1 0 0 0 1	
5.154E-04	1.290E-01	40	E003	2 2 1 1 2	
5.194E-04	1.300E-01	ns	G083	0 0 0 0 1	pH 5.5
3.196E-04	8.000E-02	ns	K444	0 0 0 0 0	
3.981E-04	9.964E-02	ns	R427	0 0 0 0 0	

2065. $C_{10}H_{10}N_4O_2S$

Sulfapyrazine
Sulphapyrazine

RN: 116-44-9 **MP** (°C)**:** 255
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2066. $C_{10}H_{10}N_4O_2S$
5-Sulfanilamidopyrimidine
5-Sulfapyrimidine
Sulfanilamide, *N*1-5-pyrimidinyl-
RN: 17103-48-9 **MP** (°C)**:**
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.916E-04	9.800E-02	37	R046	1 2 1 1 1	

2067. $C_{10}H_{10}N_4O_2S$
4-Sulfanilamidopyrimidine
4-Sulfapyrimidine
Sulfanilamide, *N*1-4-pyrimidinyl-
RN: 599-82-6 **MP** (°C)**:**
MW: 250.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.414E-02	3.540E+00	37	R045	1 2 1 1 2	

2068. $C_{10}H_{10}N_4O_4S$
5-Sulfanilamidouracil
Benzenesulfonamide, 4-amino-*N*-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)-
RN: 6912-98-7 **MP** (°C)**:**
MW: 282.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.722E-03	4.860E-01	37	R045	1 2 1 1 0	

2069. $C_{10}H_{10}O$
Benzalacetone
4-Phenyl-3-buten-2-one
Methyl styryl ketone
RN: 122-57-6 **MP** (°C)**:**
MW: 146.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-03	1.398E+00	25	R070	0 0 0 0 0	

2070. $C_{10}H_{10}O_2$
p-Acetylacetophenone
Ethanone, 1,1′-(1,4-phenylene)*bis*-
RN: 1009-61-6 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-05	6.309E-03	25	C316	0 0 0 0 0	0.1M NaCl

2071. $C_{10}H_{10}O_2$
Methyl cinnamate
2-Propenoic acid
3-Phenyl-, methyl ester
RN: 103-26-4 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.055E-01	25	R070	0 0 0 0 0	

2072. $C_{10}H_{10}O_2$
trans-α-Methyl-cinnamic acid
α-Methyl-*trans*-zimtsaeure
RN: 1895-97-2 **MP** (°C)**:**
MW: 162.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.399E-03	1.200E+00	h	F300	0 0 0 0 1	

2073. $C_{10}H_{10}O_4$
Dimethyl *o*-phthalate
RN: **MP** (°C)**:** 5.5 C
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.802E-02	3.500E+00	25	S417	0 0 0 0 0	

2074. $C_{10}H_{10}O_4$
Ferulic acid
3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid
4-Hydroxy-3-methoxycinnamic acid
RN: 1135-24-6 **MP** (°C)**:** 169 C
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.935E-03	5.700E-01	15	M461	0 0 0 0 0	
4.017E-03	7.800E-01	25	M461	0 0 0 0 0	
4.738E-03	9.200E-01	30	M461	0 0 0 0 0	
9.063E-03	1.760E+00	40	M461	0 0 0 0 0	
1.128E-02	2.190E+00	50	M461	0 0 0 0 0	

2075. $C_{10}H_{10}O_4$
Acetyl-*r*-mandelic acid
(R)(–)*O*-Acetylmandelic acid
[R]-[–]-α-(Acetoxy)phenylacetic acid
O-Acetylmandelic acid
RN: 5438-68-6 **MP** (°C)**:**
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.919E-02	5.668E+00	0	A043	1 2 1 1 1	
2.919E-02	5.668E+00	0	L035	1 2 2 1 1	
3.478E-02	6.754E+00	10	A043	1 2 1 1 1	
3.478E-02	6.754E+00	10	L035	1 2 2 1 1	
3.884E-02	7.543E+00	15	A043	1 2 1 1 1	
3.884E-02	7.543E+00	15	L035	1 2 2 1 1	
4.897E-02	9.509E+00	20	A043	1 2 1 1 1	
4.897E-02	9.509E+00	20	L035	1 2 2 1 1	
5.804E-02	1.127E+01	25	A043	1 2 1 1 2	
5.804E-02	1.127E+01	25	L035	1 2 2 1 2	
7.060E-02	1.371E+01	30	A043	1 2 1 1 2	
7.060E-02	1.371E+01	30	L035	1 2 2 1 2	
1.005E-01	1.951E+01	35	A043	1 2 1 1 2	
1.587E-01	3.082E+01	40	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	L035	1 2 2 1 2	
6.125E-01	1.189E+02	50	A043	1 2 1 1 2	
6.125E-01	1.189E+02	50	L035	1 2 2 1 2	

2076. $C_{10}H_{10}O_4$
Dimethyl phthalate
1,2-Benzenedicarboxylic acid, dimethyl ester
Fermine
Unimoll DM
Mipax
Palatinol M
RN: 131-11-3 **MP** (°C)**:** 5.5
MW: 194.19 **BP** (°C)**:** 283.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-02	4.292E+00	20	L300	2 1 0 2 2	
4.087E-02	7.937E+00	20.00	D343	0 0 0 0 0	
2.317E-01	4.500E+01	25	F067	1 0 2 2 2	*sic*
2.307E-02	4.480E+00	c	F070	1 0 0 0 0	
1.566E-02	3.041E+00	ns	F014	0 0 0 0 2	
2.052E-02	3.984E+00	ns	H069	0 0 1 1 1	
2.214E-02	4.300E+00	rt	M161	0 0 0 0 1	

2077. $C_{10}H_{10}O_4$
Meconin
Mekonin
RN: 569-31-3 **MP** (°C)**:** 102
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.287E-02	2.500E+00	25	F300	1 0 0 0 0	
2.420E-02	4.700E+00	100	F300	1 0 0 0 1	

2078. $C_{10}H_{10}O_4$
Acetylsalicylic acid, methyl ester
Methyl 2-acetoxybenzoate
Benzoic acid, 2-(acetyloxy)-, methyl ester
RN: 580-02-9 **MP** (°C)**:** 48
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-02	2.810E+00	21	N335	0 0 0 0 0	
1.679E-02	3.260E+00	37	G430	0 0 0 0 0	pH 4.5

2079. $C_{10}H_{10}O_4$
Terephthalate acid dimethyl ester
Terephthalsaeure-dimethyl ester
1,4-Benzenedicarboxylic acid dimethyl ester
Terephthalic acid
Dimethyl terephthalate
Dimethyl 1,4-Benzenedicarboxylate
RN: 120-61-6 **MP** (°C)**:** 140
MW: 194.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-04	3.282E-02	25	C316	0 0 0 0 0	0.1M NaCl
1.540E-02	2.991E+00	h	F070	1 0 0 0 1	

2080. $C_{10}H_{10}O_5$
Opianic acid
Opiansaeure
RN: 519-05-1 **MP** (°C)**:** 150
MW: 210.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.189E-02	2.500E+00	20	F300	1 0 0 0 1	
8.088E-02	1.700E+01	h	F300	0 0 0 0 1	

2081. $C_{10}H_{11}ClO_3$
Mecoprop
2-(4-Chloro-2-methylphenoxy)propionic acid
2-(2-Methyl-4-chlorophenoxy)propionic acid
2-(MCPP)
RN: 93-65-2 **MP** (°C)**:** 93
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-03	6.200E-01	20	B185	0 0 0 0 0	
2.795E-03	6.000E-01	20	B200	1 0 0 0 2	
2.887E-03	6.196E-01	20	M061	1 0 0 0 1	
2.888E-03	6.200E-01	20	M161	1 0 0 0 2	
4.170E-03	8.950E-01	25	B164	1 0 1 1 2	
4.170E-03	8.950E-01	25	B185	0 0 0 0 0	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.050E-04	4.400E-02	ns	B185	0 0 0 0 0	
2.888E-03	6.200E-01	ns	L024	1 0 0 0 2	
3.802E-03	8.161E-01	ns	R427	0 0 0 0 0	

2082. $C_{10}H_{11}ClO_3$
4-(4-Chlorophenoxy)butyric acid
4-(4-CPB)
RN: 3547-07-7 **MP** (°C)**:**
MW: 214.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.125E-04	1.100E-01	25	B164	1 0 1 1 2	

2083. $C_{10}H_{11}Cl_3O_2$
2,3,6-Trichlorobenzyloxypropanol
1-Propanol, 3-[(2,3,6-trichlorobenzyl)oxy]-
RN: 1591-82-8 **MP** (°C)**:**
MW: 269.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.708E-04	7.300E-02	25	B185	0 0 0 0 0	
2.708E-04	7.300E-02	25	B200	1 0 0 0 1	

2084. $C_{10}H_{11}FN_2O_6$
1,3-bis(Acetoxymethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1,3-bis(Acetoxymethyl)-5-fluorouracil
RN: 66542-48-1 **MP** (°C)**:** 105–106
MW: 274.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.568E-02	4.300E+00	22	B321	0 0 0 0 0	pH 4.0

2085. $C_{10}H_{11}F_3N_2O$
Fluometuron
1,1-Dimethyl-3-(α,α,α-trifluoro-*m*-tolyl)urea
RN: 2164-17-2 **MP** (°C)**:** 163
MW: 232.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.061E-01	20	B179	0 0 0 0 0	
4.522E-04	1.050E-01	20	M161	1 0 0 0 2	
3.661E-04	8.500E-02	24	C105	2 1 2 2 2	
3.876E-04	9.000E-02	25	B200	1 0 0 0 1	
3.876E-04	9.000E-02	25	G036	1 0 0 0 1	
3.876E-04	9.000E-02	25	M061	1 0 0 0 1	

2086. $C_{10}H_{11}F_3N_2O_3S$
Fluoridamid
Acetamide, *N*-{4-methyl-3-{{(trifluoromethyl)sulfonyl}amino}phenyl}-
Sustar
MBR6033
RN: 47000-92-0 **MP** (°C)**:** 182–184
MW: 296.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.388E-04	1.300E-01	22	G307	0 0 0 0 0	

2087. $C_{10}H_{11}NO$
N-Methylcinnamide
2-Propenamide, *N*-methyl-3-phenyl-
RN: 2757-10-0 **MP** (°C)**:**
MW: 161.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-02	2.112E+00	ns	H350	0 0 0 0 0	

2088. $C_{10}H_{11}NOS$
m-Isopropoxyphenyl isothiocyanate
3-Isopropoxyphenyl isothiocyanate
RN: 3528-90-3 **MP** (°C)**:**
MW: 193.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	9.084E-02	25	K032	2 2 0 1 2	

2089. $C_{10}H_{11}NO_2S$
2-Phenylthiazolidine-4-carboxylic acid
4-Thiazolidinecarboxylic acid, 2-phenyl-
RN: 42607-21-6 **MP** (°C)**:** 166–168
MW: 209.27 **BP** (°C)**:** 433.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	9.417E-01	21	B414	1 0 0 1 1	partial decomposition

2090. $C_{10}H_{11}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-methyl-
RN: 106231-50-9 **MP** (°C)**:** 111
MW: 193.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-02	3.700E+00	22	B427	1 0 0 1 1	in 0.01M HCl
1.915E-02	3.700E+00	22	N317	1 1 2 1 2	

2091. $C_{10}H_{11}NO_3$
p-Acetoxy-acetanilide
p-Acetoxyacetanilide
Acetaminophen acetate
Acetyl acetaminophen
RN: 2623-33-8 **MP** (°C)**:** 153
MW: 193.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.656E-03	3.200E-01	25	B010	1 1 1 1 0	
1.237E-02	2.390E+00	25	E016	1 1 1 1 2	
1.139E-02	2.200E+00	25	M333	1 1 0 0 2	
1.760E-02	3.400E+00	37	D029	0 0 0 0 0	

2092. $C_{10}H_{11}NO_3S$
4-Thiazolidinecarboxylic acid, 2-(4-hydroxyphenyl)-
4-Thiazolidinecarboxylic acid, 2-(*p*-hydroxyphenyl)-
RN: 69588-11-0 **MP** (°C)**:**
MW: 225.27 **BP** (°C)**:** 507.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-03	1.577E+00	21	B414	1 0 0 1 1	fast decomposition

2093. $C_{10}H_{11}NO_3S$
2-(2-Hydroxyphenyl)-4-thiazolidinecarboxylic acid
4-Thiazolidinecarboxylic acid, 2-(2-hydroxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-hydroxyphenyl)
RN: 72678-82-1 **MP** (°C)**:**
MW: 225.27 **BP** (°C)**:** 418.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	4.731E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2094. $C_{10}H_{11}NO_4$
Methyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl methyl ester
Acetanilide, 4′-hydroxy-, methyl carbonate (ester)
RN: 17321-62-9 **MP** (°C)**:** 115.5–116.5
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.868E-02	6.000E+00	37	D029	0 0 0 0 0	

2095. $C_{10}H_{11}NO_4$
O-(Acetoxymethyl) salicylamide
2-[(Acetyloxy)methoxy]-benzamide
Benzamide, 2-[(acetyloxy)methoxy]-
O-Acetoxymethyl methyl salicylamide
RN: 102273-25-6 **MP** (°C)**:** 92.5
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.39E-02	>5.00E+00	23	B328	1 2 2 1 1	pH 4
2.390E-02	5.000E+00	23	B328	0 0 0 0 0	

2096. $C_{10}H_{11}NO_4$
Carbobenzoxyglycine
N-Carbobenzyloxyglycine
N-CBZ-glycine
Benzyloxycarbonyl glycine
RN: 1138-80-3 **MP** (°C)**:**
MW: 209.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.180E-02	4.560E+00	25.1	N026	0 0 0 0 0	
2.170E-02	4.539E+00	25.1	N027	1 1 2 2 2	

2097. $C_{10}H_{11}NO_5$
Acido D-feniltartrammico tartranilico
RN: **MP** (°C)**:** 194
MW: 225.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	2.774E+01	17.40	C070	1 2 2 1 2	

2098. $C_{10}H_{11}NO_6$
Acido *p*-ossifeniltartrammico
RN: **MP** (°C)**:** 218
MW: 241.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-01	4.045E+01	14	C071	1 2 0 1 2	

2099. $C_{10}H_{11}N_3OS$
Methabenzthiazuron
N-2-Benzothiazolyl-*N,N′*-dimethylurea
1,3-Dimethyl-3-(2-benzothiazolyl)urea
Methyl-*N′*-methyl-*N′*-(2-benzothiazolyl)urea
Tribunil
Preparation 5633
RN: 18691-97-9 **MP** (°C)**:** 119.5
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-04	5.900E-02	20	M161	1 0 0 0 1	

2100. $C_{10}H_{11}N_3O_2S_2$
Methyl sulfathiazole
Sulfathiazol methyle
RN: 15251-46-4 **MP** (°C)**:**
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.653E-04	2.600E-01	37	D084	1 0 1 0 1	

2101. $C_{10}H_{11}N_3O_2S$
Sulfapyrrole
RN: **MP** (°C)**:**
MW: 237.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.023E-02	4.800E+00	20	F073	1 2 2 2 2	

2102. $C_{10}H_{11}N_3O_2S_2$
Sulfamethylthiazole
4-Methyl-2-sulfanilamidothiazole
2-(*p*-Aminobenzenesulfonamido)-4-methylthiazole
2-Sulfanilamido-4-methylthiazole
Aseptil 2
Ciba 3753
RN: 515-59-3 **MP** (°C)**:** 239
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.084E-04	1.100E-01	20	F073	1 2 2 2 2	
4.084E-04	1.100E-01	20	F074	1 0 0 0 2	

2103. $C_{10}H_{11}N_3O_2S_2$
*N*1-Methyl-*N*1-2-thiazolyl-sulfanilamide
*N*1-Methylsulfathiazole
RN: 51203-19-1 **MP** (°C)**:**
MW: 269.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	3.097E-01	37	K095	2 0 0 0 2	intrinsic

2104. $C_{10}H_{11}N_3O_3$
α-Semicarbazono-*p*-tolyl acetate
RN: **MP** (°C)**:**
MW: 221.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	3.097E-01	25	A066	1 0 1 1 1	

2105. $C_{10}H_{11}N_3O_3S$
Sulfamethoxazole
4-Amino-*N*-(5-methyl-3-isoxazolyl)benzenesulfonamide
Cotrimoxazole
Septra
Bactrim
Cotrim
RN: 723-46-6 **MP** (°C)**:** 167
MW: 253.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.810E-01	25	D308	0 0 0 0 0	pH 3.22
1.730E-03	4.383E-01	25	F415	0 0 0 0 0	Average

(*continued*)

2105. $C_{10}H_{11}N_3O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-03	3.723E-01	25	M440	0 0 0 0 0	
1.974E-03	5.000E-01	25	R025	0 0 0 0 0	
1.488E-03	3.770E-01	32	D308	0 0 0 0 0	pH 4.0
1.824E-03	4.620E-01	37	D308	0 0 0 0 0	pH 3.43
2.408E-03	6.100E-01	37	H120	1 1 1 1 1	normal saline
2.480E-03	6.281E-01	37	K095	2 0 0 0 2	intrinsic
5.527E-03	1.400E+00	37	M321	1 0 0 0 2	intrinsic
1.540E-03	3.900E-01	amb	L434	0 0 0 0 0	
1.540E-03	3.900E-01	amb	L437	0 0 0 0 0	
3.948E-05	1.000E-02	ns	K444	0 0 0 0 0	

2106. $C_{10}H_{11}N_5O_2S$

5-Sulfanilamido-2-aminopyrimidine

Benzenesulfonamide, 4-amino-*N*-(2-amino-5-pyrimidinyl)-

RN: 71119-38-5 **MP** (°C)**:**

MW: 265.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-04	8.300E-02	37	R046	1 2 1 1 1	

2107. $C_{10}H_{12}$

Tetralin

1,2,3,4-Tetrahydronaphthalene

RN: 119-64-2 **MP** (°C)**:** –31.0

MW: 132.21 **BP** (°C)**:** 207.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E-04	4.500E-02	20	B356	0 0 0 0 0	
3.532E-04	4.670E-02	28	B348	2 1 2 2 2	
1.513E-03	2.000E-01	150	J023	1 1 2 2 0	
3.026E-03	4.000E-01	200	J023	1 1 2 2 0	
3.026E-02	4.000E+00	250	J023	1 1 2 2 0	
3.236E-04	4.278E-02	ns	D001	0 0 0 0 2	

2108. $C_{10}H_{12}BrCl_2O_3PS$

Bromophos-ethyl
O-(4-Bromo-2,5-dichlorophenyl) *O,O*-diethyl phosphorothioate
Nexagan
Filariol

RN: 4824-78-6 **MP** (°C)**:**
MW: 394.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
8.629E-07	3.400E-04	20	B324	0 0 0 0 0	
8.628E-07	3.400E-04	20	B324	0 0 0 0 0	
7.613E-06	3.000E-03	20	F311	1 2 2 2 1	
5.075E-06	2.000E-03	20	W312	1 0 0 0 0	
1.269E-06	5.001E-04	30	B324	0 0 0 0 0	
1.269E-06	5.000E-04	30	B324	0 0 0 0 0	
5.075E-06	2.000E-03	ns	E050	0 0 0 0 0	
5.075E-06	2.000E-03	rt	M161	0 0 0 0 0	

2109. $C_{10}H_{12}ClNO_2$

Chloro-IPC
Furloe
Taterpex
Chlorpropham
Isopropyl *m*-chlorocarbanilate

RN: 101-21-3 **MP** (°C)**:** 38
MW: 213.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.055E-04	1.080E-01	20	B185	0 0 0 0 0	
3.744E-04	8.000E-02	25	G099	1 0 0 1 0	
3.744E-04	8.000E-02	25	G319	0 0 0 0 0	
4.165E-04	8.900E-02	25	M161	1 0 0 0 1	
3.744E-04	8.000E-02	ns	B185	0 0 0 0 0	
4.119E-04	8.800E-02	ns	B200	0 0 0 0 1	
3.744E-04	8.000E-02	ns	F035	0 0 0 0 0	
4.119E-04	8.800E-02	ns	H042	0 0 0 0 1	
3.744E-04	8.000E-02	ns	M061	0 0 0 0 1	
3.548E-04	7.581E-02	ns	M163	0 0 0 0 0	EFG
5.055E-04	1.080E-01	ns	N013	0 0 0 0 2	

2110. $C_{10}H_{12}ClNO_2$
Baclofen
Lioresal
β-(Aminomethyl)-*p*-chlorohydrocinnamic acid
RN: 1134-47-0 **MP** (°C)**:**
MW: 213.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-02	4.549E+00	25	M374	1 0 2 1 2	

2111. $C_{10}H_{12}ClN_3O_2$
Tranid
3-Chloro-6-cyanonorbornanone-2-oxime-*O,N*-methylcarbamate
RN: 15271-41-7 **MP** (°C)**:** 143.5
MW: 241.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.259E-03	1.996E+00	ns	M061	0 0 0 0 0	

2112. $C_{10}H_{12}ClN_3O_3S$
Quinethazone
7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinazolinesulfonamide
Hydromox
CL 36010
Aquamox
RN: 73-49-4 **MP** (°C)**:** 251
MW: 289.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-04	1.500E-01	25	A081	1 0 1 1 0	EFG

2113. $C_{10}H_{12}ClN_5O_2$
2-Chloro-2′,3′-dideoxyadenosine
2-CIDDA
RN: 114849-58-0 **MP** (°C)**:**
MW: 269.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.745E-03	1.010E+00	25	A336	0 0 0 0 0	

2114. $C_{10}H_{12}Cl_2O$

2,4-Dichloro-6-butyl-phenol
Phenol, 2-butyl-4,6-dichloro-
RN: 91399-13-2 **MP** (°C)**:**
MW: 219.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.259E-02	25	B316	0 0 0 0 0	

2115. $C_{10}H_{12}Cl_3O_2PS$

Trichloronate
Trichloronat
Ethyl *O*-(2,4,5-trichlorophenyl) ethylphosphonothioate
Agritox
Bay 37289
RN: 327-98-0 **MP** (°C)**:**
MW: 333.60 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
1.769E-06	5.901E-04	20	B300	2 1 1 1 2	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
1.499E-04	5.000E-02	20	M161	1 0 0 0 1	*sic*
3.208E-06	1.070E-03	30	B324	0 0 0 0 0	
3.207E-06	1.070E-03	30	B324	0 0 0 0 0	

2116. $C_{10}H_{12}N_2O_2$

Acetone *N*-(phenylcarbamoyl)oxime
Acetone oxime *N*-phenylcarbamate
Proxypham
RN: **MP** (°C)**:** 109.5
MW: 192.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.601E-03	5.000E-01	ns	M061	0 0 0 0 2	approximate

2117. $C_{10}H_{12}N_2O_3$

Barbituric-2-14C acid, 5,5-diallyl
RN: 112599-90-3 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.381E-03	1.745E+00	25	P350	0 0 0 0 0	intrinsic

2118. $C_{10}H_{12}N_2O_3$
Allobarbital
5,5-Diallylbarbituric acid
RN: 52-43-7 **MP** (°C)**:** 171
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.003E-03	1.250E+00	20	J030	1 2 2 2 2	
7.193E-03	1.498E+00	25	A023	1 0 0 1 2	
8.500E-03	1.770E+00	25	G003	1 1 1 1 1	pH 4.7
8.650E-03	1.801E+00	25	V033	2 0 1 1 2	
8.700E-03	1.812E+00	25.00	T303	1 0 0 0 1	
9.250E-03	1.926E+00	30	G014	1 1 1 1 0	EFG
9.200E-03	1.916E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
9.200E-03	1.916E+00	30	K108	1 2 2 0 1	
1.150E-02	2.394E+00	35	A023	1 0 0 1 2	
1.110E-02	2.311E+00	35.00	T303	1 0 0 0 2	
1.215E-02	2.530E+00	37	J030	1 2 2 2 2	
1.200E-02	2.499E+00	37	K121	1 2 1 2 1	0.1N HCl
1.675E-02	3.488E+00	40	A023	1 0 0 1 2	
1.370E-01	2.853E+01	40	N008	1 0 1 1 2	*sic*
1.690E-02	3.519E+00	45.00	T303	1 0 0 0 2	
7.036E-03	1.465E+00	ns	T003	0 0 0 0 2	

2119. $C_{10}H_{12}N_2O_3S$
Bentazon
2,1,3-Benzothiadiazin-4(3H)-one
Thiadiazinol
Basagran 4E
Adagio
BAS 351H
RN: 25057-89-0 **MP** (°C)**:** 138.0
MW: 240.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-03	5.000E-01	20	M161	1 0 0 0 2	
2.080E-03	4.998E-01	ns	B100	0 0 0 0 0	
3.329E-03	8.000E-01	ns	M110	0 0 0 0 0	EFG

2120. $C_{10}H_{12}N_2O_4$
Stavudine
1-(2,3-Dideoxy-β-D-glycero-pent-2-enofuranosyl)thymine
BMY-27857
d4T
Zerit
3′-Deoxy-2′-thymidinene
RN: 3056-17-5 **MP** (°C)**:** 159–160
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-01	7.519E+01	20.5	M439	0 0 0 0 0	
3.791E-01	8.500E+01	24.8	M439	0 0 0 0 0	
4.238E-01	9.502E+01	29.4	M439	0 0 0 0 0	
4.668E-01	1.047E+02	33.2	M439	0 0 0 0 0	
5.563E-01	1.247E+02	38.4	M439	0 0 0 0 0	
3.702E-01	8.300E+01	ns	K444	0 0 0 0 0	
3.418E-01	7.664E+01	ns	S469	0 0 0 0 0	

2121. $C_{10}H_{12}N_2O_4S$
*N*1,*N*4-Diacetylsulfanilamide
*N*4-Acetylsulphacetamide
RN: 5626-90-4 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.389E-03	2.150E+00	37	L091	1 0 0 0 2	pH 5.5

2122. $C_{10}H_{12}N_2O_5$
D-Monofeniltartramide tartranilamide
RN: **MP** (°C)**:** 226
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-02	4.704E+00	21.50	C070	1 2 2 1 2	

2123. $C_{10}H_{12}N_2O_5$

2,4-Dinitro-6-*sec*-butylphenol
Dinoseb
4,6-Dinitro-2-*S*-butylphenol
Phenol, 4,6-dinitro-2-*sec*-butyl-

RN: 88-85-7 **MP** (°C)**:** 38
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.165E-04	5.200E-02	25	B200	1 0 0 0 1	
2.165E-04	5.200E-02	25	G319	0 0 0 0 0	
3.053E-03	7.335E-01	25	M061	1 0 0 0 2	
4.159E-03	9.990E-01	ns	B100	0 0 0 0 0	
2.081E-04	5.000E-02	ns	B185	0 0 0 0 0	
1.413E-03	3.393E-01	ns	M163	0 0 0 0 0	EFG
2.165E-04	5.200E-02	ns	V414	0 0 0 0 0	
4.163E-04	1.000E-01	rt	M161	0 0 0 0 2	

2124. $C_{10}H_{12}N_2O_5S$

7-Aminocephalosporanic acid
7-ACA

RN: 957-68-6 **MP** (°C)**:**
MW: 272.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.901E-04	2.696E-01	1.29	W417	0 0 0 0 0	
1.070E-03	2.914E-01	5.19	W417	0 0 0 0 0	
1.130E-03	3.076E-01	8.29	W417	0 0 0 0 0	
1.255E-03	3.416E-01	12.19	W417	0 0 0 0 0	
1.367E-03	3.723E-01	17.59	W417	0 0 0 0 0	
1.504E-03	4.096E-01	22.99	W417	0 0 0 0 0	
1.627E-03	4.429E-01	27.99	W417	0 0 0 0 0	

2125. $C_{10}H_{12}N_3O_3PS_2$

Azinphos-methyl
Guthion
S-(3,4-Dihydro-4-oxobenzo[d][1,2,3]triazin-3-ylmethyl) *O,O*-dimethyl phosphorodithioate
Methyl gusathion

RN: 86-50-0 **MP** (°C)**:** 74
MW: 317.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.994E-05	9.501E-03	10	B324	0 0 0 0 0	
2.994E-05	9.500E-03	10	B324	0 0 0 0 0	
4.412E-05	1.400E-02	15	A087	1 0 0 1 0	
6.587E-05	2.090E-02	20	B300	2 1 1 1 2	

(*continued*)

2125. $C_{10}H_{12}N_3O_3PS_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.587E-05	2.090E-02	20	B324	0 0 0 0 0	
6.586E-05	2.090E-02	20	B324	0 0 0 0 0	
9.454E-05	3.000E-02	20	M061	1 0 0 0 1	
9.139E-05	2.900E-02	25	A087	1 0 0 1 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.481E-04	4.700E-02	35	A087	1 0 0 1 0	
8.913E-05	2.828E-02	ns	R427	0 0 0 0 0	
1.040E-04	3.300E-02	rt	M161	0 0 0 0 1	

2126. $C_{10}H_{12}N_4$

6,7-Diethylpteridine

RN: **MP** (°C)**:** 52

MW: 188.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.641E-01	1.250E+02	20	A019	2 2 1 1 0	

2127. $C_{10}H_{12}N_4O$

2-Hydroxy-6,7-diethylpteridine
2-Hydroxy-6:7-diethylpteridine
4-Hydroxy-6,7-diethylpteridine
4-Hydroxy-6:7-diethylpteridine

RN: 90870-76-1 **MP** (°C)**:**

MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.494E+00	20	A019	2 2 1 1 2	
5.434E-03	1.110E+00	20	A019	2 2 1 1 2	

2128. $C_{10}H_{12}N_4O_2$

2,4-Dihydroxy-6,7-diethylpteridine
2,4-Dihydroxy-6:7-diethylpteridine

RN: 113222-29-0 **MP** (°C)**:** 218

MW: 220.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.124E-03	9.083E-01	20	A019	2 2 1 1 2	

2129. $C_{10}H_{12}N_4O_2$
1H-Pyrazolo[3,4-d]pyrimidine, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-
2-Tetrahydropuran-4-allopurinyl ether
RN: 52717-52-9 **MP** (°C)**:**
MW: 220.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-02	3.640E+00	ns	H067	0 0 0 0 0	

2130. $C_{10}H_{12}N_4O_2S$
Sulfaethidole
Ethyl thiodiazole
Sulfaethylthiadiazole
Thiodiazolique ethyle
RN: 94-19-9 **MP** (°C)**:** 188
MW: 252.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.522E-04	2.150E-01	20	F073	1 2 2 2 2	
1.288E-02	3.250E+00	37	B046	1 0 2 2 2	pH 5
1.585E-03	4.000E-01	37	D084	1 0 1 0 1	

2131. $C_{10}H_{12}N_4O_3$
1-Butyryloxymethyl allopurinol
Butanoic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-21-5 **MP** (°C)**:** 224–226
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.482E-03	3.500E-01	22	B322	0 0 0 0 0	

2132. $C_{10}H_{12}N_4O_3$
2′,3′-Dideoxyinosine
Videx
Didanosine
CCRIS 805
CCRIS 805Didanosine
RN: 69655-05-6 **MP** (°C)**:** 175
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.614E-02	1.090E+01	4	A337	0 0 0 0 0	
1.156E-01	2.730E+01	25	A337	0 0 0 0 0	
1.270E-01	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic
1.156E-01	2.730E+01	ns	K444	0 0 0 0 0	
1.125E-01	2.657E+01	ns	S469	0 0 0 0 0	

2133. $C_{10}H_{12}N_4O_3$
2-Butyryloxymethyl allopurinol
Butanoic acid, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-22-6 **MP** (°C)**:** 182–183
MW: 236.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.500E+00	22	B322	0 0 0 0 0	

2134. $C_{10}H_{12}N_4O_4$
2′-Deoxy-inosine
2[-Deoxyinosine
Deoxyinosine
RN: 890-38-0 **MP** (°C)**:**
MW: 252.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.301E-02	8.326E+00	25.02	T420	0 0 0 0 0	

2135. $C_{10}H_{12}N_4O_5$
Inosine
Inosin
Hypoxanthine ribonucleoside
RN: 58-63-9 **MP** (°C)**:** 212dec
MW: 268.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.871E-02	1.575E+01	20	D041	1 0 0 0 1	
5.890E-02	1.580E+01	20	F300	1 0 0 0 2	
5.888E-02	1.579E+01	ns	R427	0 0 0 0 0	

2136. $C_{10}H_{12}N_4O_6$
2,4,6-Trinitrodiethylaniline
2-4-6-Trinitrodiethylaniline
RN: 106415-21-8 **MP** (°C)**:**
MW: 284.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.759E-04	5.000E-02	50	D067	1 2 0 0 0	
7.037E-04	2.000E-01	100	D067	1 2 0 0 1	

2137. $C_{10}H_{12}N_5O_6P$
Adenosine 3′:5′-monophosphate
Adenosine, cyclic 3′,5′-(hydrogen phosphate)
4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, adenosine deriv
RN: 60-92-4 **MP** (°C)**:**
MW: 329.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-02	7.769E+00	20	D034	0 0 0 0 0	pH 7.0

2138. $C_{10}H_{12}N_6O_2S$
2-*S*-Cysteinyl-4,6-*bis*-(dimethylamino)-*s*-triazine
RN: **MP** (°C)**:** 173
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.991E-03	2.240E+00	25	C051	1 2 1 1 2	pH 7

2139. $C_{10}H_{12}O$
Estragole
1-Methoxy-4-(2-propen-1-yl)benzene
Chavicyl methyl ether
4-Allylanisole
Tarragon
RN: 140-67-0 **MP** (°C)**:** <25
MW: 148.21 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.778E-01	25	I019	1 0 1 2 2	

2140. $C_{10}H_{12}O$
Anethole
Methoxy-4-propenylbenzene
Propenylanisole
p-Propenylanisole
Anise camphor
Isoestragole
RN: 104-46-1 **MP** (°C)**:** 21.4
MW: 148.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.482E-01	25	D407	1 0 2 2 2	
7.490E-04	1.110E-01	25	I019	1 0 1 2 2	
7.413E-04	1.099E-01	ns	S460	0 0 0 0 0	

2141. $C_{10}H_{12}O$
5,6,7,8-Tetrahydro-2-naphthol
5,6,7,8-Tetrahydro-naphthol-(2)
RN: 1125-78-6 **MP** (°C)**:** 56.5
MW: 148.21 **BP** (°C)**:** 275.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.500E+00	20	F300	1 0 0 0 1	

2142. $C_{10}H_{12}O_2$
Eugenol
1-Allyl-3-methoxy-4-hydroxybenzene
2-Methoxy-4-allylphenol
2-Methoxy-4-(2-propenyl)phenol
4-Allylguaiacol
Allylguaiacol
RN: 97-53-0 **MP** (°C)**:** 15
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-02	2.463E+00	25	I019	1 0 1 2 2	
4.020E-02	6.601E+00	37	E028	1 0 1 1 2	

2143. $C_{10}H_{12}O_2$
Ethyl 2-phenylacetate
Phenylacetic acid ethyl ester
Ethyl benzeneacetate; ethyl phenacetate
NSC 8894
NSC 406259
Ethyl phenylacetate
RN: 101-97-3 **MP** (°C)**:**
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-03	1.478E+00	25	D407	1 0 2 2 2	
8.995E-03	1.477E+00	ns	S460	0 0 0 0 0	

2144. $C_{10}H_{12}O_2$
β-Phenylbutyric acid
3-Phenyl-*n*-butyric acid
RN: 4593-90-2 **MP** (°C)**:** 38
MW: 164.21 **BP** (°C)**:** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	9.254E+00	30	D033	2 2 1 2 2	
7.013E-02	1.152E+01	40	D033	2 2 1 2 2	

2145. $C_{10}H_{12}O_2$

b-Phenylethanol acetate
Phenylethyl ethanoate
b-Phenylethyl acetate
2-Phenethyl acetate; 2-phenylethyl acetate
Benzylcarbinyl acetate
NSC 71927

RN: 103-45-7 **MP** (°C)**:**
MW: 164.21 **BP** (°C)**:** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.135E+00	25	D407	1 0 2 2 2	
1.300E-02	2.135E+00	ns	S460	0 0 0 0 0	

2146. $C_{10}H_{12}O_2$

2,4,6-Trimethylbenzoic acid
Mesitylenecarboxylic acid

RN: 480-63-7 **MP** (°C)**:** 154
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-03	7.225E-01	ns	C014	0 2 0 1 1	

2147. $C_{10}H_{12}O_2$

n-Propyl benzoate
Propyl benzoate
Benzoicacidpropyl ester

RN: 2315-68-6 **MP** (°C)**:** –51
MW: 164.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E-03	2.514E-01	20	H301	0 0 0 0 0	

2148. $C_{10}H_{12}O_3$

Anisyl acetate
4-Methoxybenzyl acetate
Benzenemethanol, 4-methoxy-, acetate

RN: 104-21-2 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	1.982E+00	25	D407	1 0 2 2 2	

2149. $C_{10}H_{12}O_3$
Propylparaben
Pr-paraben
Propyl *p*-hydroxybenzoic acid
Propyl 4-hydroxybenzoate
Propyl paraben
RN: 94-13-3 **MP** (°C)**:** 96.5
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.050E-03	3.694E-01	15	B355	0 0 0 0 0	
1.172E-03	2.112E-01	15	M352	1 1 1 1 2	
2.410E-03	4.343E-01	20	B355	0 0 0 0 0	
2.055E-03	3.703E-01	25	A059	1 0 1 1 1	
2.570E-03	4.631E-01	25	B355	0 0 0 0 0	
2.773E-03	4.998E-01	25	D081	1 2 2 1 2	
1.990E-03	3.586E-01	25	D339	0 0 0 0 0	
1.778E-03	3.205E-01	25	F322	2 0 1 1 0	EFG
1.844E-03	3.323E-01	25	M352	1 1 1 1 2	
2.775E-03	5.000E-01	25	O027	1 0 1 0 0	
2.863E-03	5.160E-01	25	P013	0 0 0 0 0	
2.300E-03	4.145E-01	27	B129	2 2 2 2 1	
2.443E-03	4.403E-01	30	A059	1 0 1 1 1	
2.053E-03	3.700E-01	30	M325	1 0 0 0 1	
3.054E-03	5.503E-01	35	A059	1 0 1 1 1	
3.403E-03	6.132E-01	39.3	G302	2 2 2 2 0	EFG
4.053E-03	7.303E-01	40	A059	1 0 1 1 1	
3.925E-03	7.073E-01	40	M352	1 1 1 1 2	
6.492E-03	1.170E+00	50	M352	1 1 1 1 2	
1.515E-03	2.729E-01	ns	B404	0 2 1 1 0	

2150. $C_{10}H_{12}O_4$
Cantharidin
Dimethyl-3,6-epoxyperhydrophthalic anhydride
Cantharides
Hexahydro-3α,7α-dimethyl-4β,7β-epoxyisobenzofuran-1,3-dione
Spanish fly
RN: 56-25-7 **MP** (°C)**:**
MW: 196.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	3.000E-02	20	F300	1 0 0 0 0	
3.058E-01	6.000E+01	100	F300	1 0 0 0 0	
1.514E-04	2.970E-02	ns	R427	0 0 0 0 0	

2151. $C_{10}H_{12}O_5$

Propyl gallate
3,4,5-Trihydroxybenzoic acid propyl ester
Gallic acid propyl ester
Progallin P
n-propyl 3,4,5-trihydroxybenzoate
Nipa 49

RN: 121-79-9 **MP** (°C)**:** 150 C
MW: 212.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-02	2.792E+00	19.99	L430	0 0 0 0 0	
1.644E-02	3.488E+00	24.99	L430	0 0 0 0 0	
1.784E-02	3.786E+00	29.99	L430	0 0 0 0 0	
3.276E-02	6.951E+00	34.99	L430	0 0 0 0 0	
4.850E-02	1.029E+01	39.99	L430	0 0 0 0 0	
7.010E-02	1.488E+01	44.99	L430	0 0 0 0 0	
2.321E-01	4.925E+01	49.99	L430	0 0 0 0 0	
1.158E-01	2.458E+01	49.99	L430	0 0 0 0 0	
6.751E-01	1.432E+02	59.99	L430	0 0 0 0 0	
1.111E+00	2.357E+02	64.99	L430	0 0 0 0 0	
5.648E-03	1.199E+00	–.0	L430	0 0 0 0 0	

2152. $C_{10}H_{12}O_8$

Dilactone
α-Oxo-β-methylol-γ-butyrolactone betrachten

RN: **MP** (°C)**:** 140
MW: 260.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.374E-02	2.439E+01	0	F023	1 1 0 0 1	unit assumed
1.900E-01	4.943E+01	25	F023	1 1 0 0 1	unit assumed
5.972E-01	1.554E+02	50	F023	1 1 0 0 2	unit assumed
1.788E+00	4.652E+02	75	F023	1 1 0 0 2	unit assumed
2.451E+00	6.377E+02	100	F023	1 1 0 0 2	unit assumed

2153. $C_{10}H_{13}ClN_2$
Chlordimeform
N′-(4-Chloro-2-methylphenyl)-*N,N*-dimethylmethanimidamide
Bermat
Fundex
Galecon
Chlorophenamidine
RN: 6164-98-3 **MP** (°C)**:** 32
MW: 196.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.373E-03	2.700E-01	20	B300	2 0 1 1 2	
1.373E-03	2.700E-01	20	B324	0 0 0 0 0	
1.372E-03	2.699E-01	20	B324	0 0 0 0 0	
1.271E-03	2.500E-01	20	M161	1 0 0 0 2	

2154. $C_{10}H_{13}ClN_2O$
Trimeturon
N′-4-Chlorophenyl-*O,N,N*-trimethylisourea
RN: 3050-27-9 **MP** (°C)**:** 147.5
MW: 212.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.289E-03	6.995E-01	ns	M061	0 0 0 0 1	

2155. $C_{10}H_{13}ClN_2O$
Chlortoluron
N′-(3-Chloro-4-methylphenyl)-*N,N*-dimethylurea
Dicuran
Chlortokem
Tolurex
RN: 15545-48-9 **MP** (°C)**:** 147.5
MW: 212.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	7.043E-02	20	B179	0 0 0 0 0	
3.291E-04	7.000E-02	20	F311	1 2 2 2 1	
3.291E-04	7.000E-02	20	M161	1 0 0 0 1	

2156. $C_{10}H_{13}ClN_2O_2$

Metoxuron
N′-(3-Chloro-4-methoxyphenyl)-*N,N*-dimethylurea
Purivel
Sulerex
Dosanex
Dosaflo

RN: 19937-59-8 **MP** (°C)**:** 125
MW: 228.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.906E-01	20	B179	0 0 0 0 0	
2.622E-03	5.996E-01	20	E048	1 2 1 1 2	
2.965E-03	6.780E-01	23	M161	0 0 0 0 2	
3.059E-03	6.995E-01	ns	B100	0 0 0 0 0	

2157. $C_{10}H_{13}ClN_2O_3S$

Chlorpropamide
*N*3-Butyl-*N*1-*p*-chlorobenzenesulfonylurea
Diabinese
Glucamide
Catanil
Diabaril

RN: 94-20-2 **MP** (°C)**:** 128
MW: 276.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.221E-03	8.913E-01	25	F415	0 0 0 0 0	
9.311E-04	2.577E-01	37	A028	1 0 2 1 2	intrinsic
9.250E-04	2.560E-01	37	A046	2 0 1 1 2	
~1.26E-03	~3.50E-01	37	B140	2 2 1 2 0	pH 1.5, form V
1.203E-03	3.330E-01	37	B140	2 2 1 2 2	pH 1.5, form I
1.384E-03	3.830E-01	37	B140	2 2 1 2 2	pH 1.5, form II
8.925E-04	2.470E-01	37	B140	2 2 1 2 2	pH 1.5, form III
1.153E-03	3.190E-01	37	B140	2 2 1 2 2	pH 1.5, form IV
>1.81E-03	>5.00E-01	ns	B404	0 2 1 1 0	
5.192E-04	1.437E-01	rt	I404	0 0 0 0 0	Average

2158. $C_{10}H_{13}Cl_2FN_2O_2S_2$
Tolylfluanid
1,1-Dichloro-*N*-((dimethylamino)sulfonyl)-1-fluoro-*N*-(4-methylphenyl)methanesulfenamide
Dichlofluanid-methyl
Euparen M
Bay 5712α
Bay 49854
RN: 731-27-1 **MP** (°C)**:** 96
MW: 347.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.570E-06	8.926E-04	ns	R427	0 0 0 0 0	
1.152E-02	4.000E+00	rt	M161	0 0 0 0 0	

2159. $C_{10}H_{13}Cl_2O_3PS$
Dichlofenthion
Diethyl *O*-dichlorophenyl phosphorothioate
Hexanema
Diclophenthion
Nemacide
TRI-VC13
RN: 97-17-6 **MP** (°C)**:**
MW: 315.16 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.774E-07	2.450E-04	25	M161	1 0 0 0 2	
7.774E-07	2.450E-04	ns	F071	0 1 2 1 2	
7.774E-04	2.450E-01	ns	M061	0 0 0 0 2	*sic*

2160. $C_{10}H_{13}FN_2O_3$
1-Pivaloyloxymethyl-5-fluorouracil
RN: **MP** (°C)**:**
MW: 228.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	2.500E+00	22	M317	1 1 1 1 1	

2161. $C_{10}H_{13}FN_2O_4$
1-Pivaloyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Pivaloyloxymethyl-5-fluorouracil
RN: 62113-42-2 **MP** (°C)**:** 158-160
MW: 244.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-03	2.300E+00	22	B321	0 0 0 0 0	pH 4.0

2162. $C_{10}H_{13}NO_2$
Phenacetin
p-Ethoxyacetanilide
p-Acetophenetidide
RN: 62-44-2 **MP** (°C)**:** 134.5
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.010E-04	5.395E-02	14	O019	1 0 0 1 2	
2.010E-03	3.603E-01	15	M352	1 1 1 1 2	
3.903E-03	6.995E-01	20	M043	1 0 0 0 0	
5.167E-03	9.261E-01	25	B434	0 0 0 0 0	
5.180E-03	9.284E-01	25	B434	0 0 0 0 0	
4.300E-02	7.706E+00	25	D044	0 0 0 0 0	
4.464E-03	8.000E-01	25	F300	1 0 0 0 0	
2.801E-03	5.020E-01	25	M333	1 1 0 0 2	
2.799E-03	5.016E-01	25	M352	1 1 1 1 2	
6.271E-03	1.124E+00	30	B434	0 0 0 0 0	
6.280E-03	1.126E+00	30	B434	0 0 0 0 0	
8.653E-03	1.551E+00	35	B434	0 0 0 0 0	
8.680E-03	1.556E+00	35	B434	0 0 0 0 0	
1.183E-02	2.120E+00	40	B434	0 0 0 0 0	
1.185E-02	2.124E+00	40	B434	0 0 0 0 0	
5.483E-03	9.828E-01	40	M352	1 1 1 1 2	
7.878E-03	1.412E+00	50	M352	1 1 1 1 2	
6.616E-02	1.186E+01	100	I315	0 0 0 0 0	
7.867E-02	1.410E+01	100	M043	1 0 0 0 2	
4.237E-03	7.594E-01	c	I315	0 0 0 0 0	
6.584E-03	1.180E+00	ns	F059	1 0 2 2 2	0.1N HCl
5.574E-03	9.990E-01	rt	D021	0 0 1 1 1	

2163. $C_{10}H_{13}NO_2$
Propham
Isopropyl carbanilate
Isopropyl-*N*-phenyl carbamate
IPC
RN: 122-42-9 **MP** (°C)**:** 87
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.580E-04	1.000E-01	25	G099	1 0 0 1 0	
1.116E-04	2.000E-02	ns	B185	0 0 0 0 0	
1.786E-04	3.200E-02	ns	B185	0 0 0 0 0	
1.395E-03	2.500E-01	ns	B200	0 0 0 0 2	
5.580E-04	1.000E-01	ns	F035	0 0 0 0 0	
1.395E-03	2.500E-01	ns	H042	0 0 0 0 2	
1.000E-03	1.792E-01	ns	M163	0 0 0 0 0	EFG
1.395E-03	2.500E-01	ns	N013	0 0 0 0 2	

2164. $C_{10}H_{13}NO_2$
Butyl nicotinate
n-Butyl nicotinate
RN: 6938-06-3 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-02	2.450E+00	32	L346	1 0 0 1 2	

2165. $C_{10}H_{13}NO_2$
Propyl-*p*-aminobenzoate
Risocaine
4-Aminobenzoic acid propyl ester
RN: 94-12-2 **MP** (°C)**:** 75.5
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.655E-03	2.966E-01	15	M352	1 1 1 1 2	
2.220E-03	3.979E-01	25	H008	0 0 0 0 0	
2.860E-03	5.125E-01	25	M352	1 1 1 1 2	
3.553E-03	6.368E-01	25	P303	0 0 0 0 0	
4.219E-03	7.561E-01	33	P303	0 0 0 0 0	
4.700E-03	8.423E-01	37	F006	1 1 2 2 2	
4.629E-03	8.297E-01	40	M352	1 1 1 1 2	
5.217E-03	9.351E-01	40	P303	0 0 0 0 0	
7.047E-03	1.263E+00	50	M352	1 1 1 1 2	
1.890E-03	3.387E-01	ns	M066	0 0 0 0 2	
1.890E-03	3.387E-01	rt	B016	0 0 1 1 2	pH 7.4

2166. $C_{10}H_{13}NO_2$
3,4-Xylyl methylcarbamate
3,4-Dimethylphenyl methylcarbamate
3,4-Dimethylphenyl *N*-methylcarbamate
MPMC
Meobal
RN: 2425-10-7 **MP** (°C)**:** 79.5
MW: 179.22 **BP** (°C)**:** 126.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.254E-03	1.300E+00	30	M161	1 0 0 0 1	

2167. $C_{10}H_{13}NO_2$
2,6-Dimethyl-4-acetaminophenol
4-Acetamido-2,6-dimethylphenol
RN: 22900-79-4 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-02	2.200E+00	25	D078	1 2 1 1 2	

2168. $C_{10}H_{13}NO_2$
Methyl *p*-dimethylaminobenzoic acid
Methyl 4-dimethylaminobenzoate
RN: 1202-25-1 **MP** (°C)**:** 371.7
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	6.093E-02	15	M352	1 1 1 1 2	
4.988E-04	8.940E-02	25	M352	1 1 1 1 2	
8.277E-04	1.483E-01	40	M352	1 1 1 1 2	
1.111E-03	1.991E-01	50	M352	1 1 1 1 2	

2169. $C_{10}H_{13}NO_2$
2,5-Dimethyl-4-acetaminophenol
4-Acetamido-2,5-dimethylphenol
RN: 69477-71-0 **MP** (°C)**:**
MW: 179.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-03	1.737E+00	25	D078	1 2 1 1 2	

2170. $C_{10}H_{13}NO_3$
o-Ethoxyphenyl *N*-methylcarbamate
1,2-Ethoxyphenyl *N*-methylcarbamate
RN: 23409-17-8 **MP** (°C)**:** 79.5
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.178E-02	2.300E+00	30	D089	2 2 0 0 0	

2171. $C_{10}H_{13}NO_3$
m-Ethoxyphenyl *N*-methylcarbamate
1,3-Ethoxyphenyl *N*-methylcarbamate
RN: 7225-96-9 **MP** (°C)**:** 57
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.403E-03	1.250E+00	30	D089	2 2 0 0 0	

2172. $C_{10}H_{13}NO_4$
Methyldopa
α-Methyldopa
Sembrina
Presinol
Sedometil
Presolisin
RN: 555-30-6 **MP** (°C)**:** ~300
MW: 211.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.734E-02	1.000E+01	ns	K444	0 0 0 0 0	

2173. $C_{10}H_{13}N_3O_2S_2$
3-Methyl-2-sulfanilamide-2,3-dihydrothiazole
Benzenesulfonamide, 4-amino-*N*-(2,3-dihydro-3-methyl-2-thiazolyl)-
RN: 51203-20-4 **MP** (°C)**:**
MW: 271.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.690E-04	1.544E-01	37	K095	2 0 0 0 2	intrinsic

2174. $C_{10}H_{13}N_3O_5S$
Nifurtimox
4-((5-Nitrofurfurylidene)amino)-3-methylthiomorpholine-1,1-dioxide
RN: 23256-30-6 **MP** (°C)**:**
MW: 287.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.149E-01	3.300E+01	ns	K444	0 0 0 0 0	

2175. $C_{10}H_{13}N_4O_3$
Spasmolysin
β-Hydroxypropyltheophylline
RN: 603-00-9 **MP** (°C)**:**
MW: 237.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E+00	2.857E+02	ns	J025	0 0 0 0 1	

2176. $C_{10}H_{13}N_5$
4-Amino-6,7-diethylpteridine
RN: **MP** (°C)**:**
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.171E-03	2.380E-01	20	A019	2 2 1 1 2	

2177. $C_{10}H_{13}N_5$
2-Amino-6,7-diethylpteridine
RN: **MP** (°C)**:**
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.110E-04	1.852E-01	20	A019	2 2 1 1 2	

2178. $C_{10}H_{13}N_5O$
2-Amino-4-hydroxy-6,7-diethylpteridine
2-Amino-4-hydroxy-6:7-diethylpteridine
RN: **MP** (°C)**:** >350
MW: 219.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-05	1.163E-02	20	A019	2 2 1 1 2	

2179. $C_{10}H_{13}N_5O$
4-Amino-2-hydroxy-6,7-diethylpteridine
4-Amino-2-hydroxy-6:7-diethylpteridine
RN: **MP** (°C)**:**
MW: 219.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.850E-04	6.250E-02	20	A019	2 2 1 1 2	

2180. $C_{10}H_{13}N_5O_2$
2′,3′-Dideoxyadenosine
DDA
RN: 4097-22-7 **MP** (°C)**:** 181–184
MW: 235.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.228E-01	2.890E+01	4	A337	0 0 0 0 0	
1.836E-01	4.320E+01	25	A337	0 0 0 0 0	

2181. $C_{10}H_{13}N_5O_3$
Deoxyadenosine
2′-Deoxyadenosine
dA
RN: 958-09-8 **MP** (°C)**:**
MW: 251.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E-02	3.573E+00	14.88	T420	0 0 0 0 0	
1.827E-02	4.590E+00	20.26	T420	0 0 0 0 0	
2.690E-02	6.759E+00	25	H061	0 0 0 0 0	
2.558E-02	6.427E+00	25.23	T420	0 0 0 0 0	
3.683E-02	9.253E+00	29.97	T420	0 0 0 0 0	
4.780E-02	1.201E+01	35.09	T420	0 0 0 0 0	

2182. $C_{10}H_{13}N_5O_4$
Zidovudine
3-Azido-3-deoxythymidine
AZT
Azidodeoxythymidine
Azidothymidine
Retrovir
RN: 30516-87-1 **MP** (°C)**:** 106–112
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.13E+00	>3.02E+02	25	B443	0 0 0 0 0	
7.521E-02	2.010E+01	ns	K444	0 0 0 0 0	
7.373E-02	1.970E+01	ns	S469	0 0 0 0 0	

2183. $C_{10}H_{13}N_5O_4$
Adenosine
Adenosin
9-B-D-Ribofuranosyl-9H-purin-6-amine adenine riboside
Adenocard
9-β-D-Ribofuranosyladenine
RN: 58-61-7 **MP** (°C)**:** 234
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	5.131E+00	25	H061	0 0 0 0 0	
2.000E-02	5.345E+00	ns	R030	0 0 0 0 0	
1.905E-02	5.092E+00	ns	R427	0 0 0 0 0	
8.232E-05	2.200E-02	rt	N015	0 0 2 2 1	*sic*

2184. $C_{10}H_{13}N_5O_4$
Guanine deoxyriboside
RN: 961-07-9 **MP** (°C)**:**
MW: 267.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E-03	1.785E+00	14.88	T420	0 0 0 0 0	
8.790E-03	2.349E+00	20.26	T420	0 0 0 0 0	
1.118E-02	2.988E+00	25.02	T420	0 0 0 0 0	
1.589E-02	4.247E+00	29.97	T420	0 0 0 0 0	
2.072E-02	5.537E+00	35.09	T420	0 0 0 0 0	

2185. $C_{10}H_{13}N_5O_5$
Guanosine
Guanosin
2-Amino-9-β-D-ribofuranosyl-9H-purine-6-(1H)-one
Guanine riboside
rG
RN: 118-00-3 **MP** (°C)**:** 250
MW: 283.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.471E-03	7.000E-01	18	F300	1 0 0 0 1	
4.300E-03	1.218E+00	25	C416	2 1 1 1 1	
1.820E-03	5.155E-01	25	H061	0 0 0 0 0	
1.073E-01	3.040E+01	100	F300	1 0 0 0 1	

2186. $C_{10}H_{14}$
Isobutylbenzene
2-Methyl-1-phenylpropane
(2-Methylpropyl)-benzene
RN: 538-93-2 **MP** (°C)**:** –51
MW: 134.22 **BP** (°C)**:** 170.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.525E-05	1.010E-02	25	P051	2 1 1 2 2	
7.525E-05	1.010E-02	25.00	P007	2 1 2 2 2	
7.525E-05	1.010E-02	ns	H123	0 0 0 0 0	

2187. $C_{10}H_{14}$
Durene
1,2,4,5-Tetramethylbenzene
Durol
RN: 95-93-2 **MP** (°C)**:** 80.0
MW: 134.22 **BP** (°C)**:** 192.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.593E-05	3.480E-03	25	K119	1 0 0 0 2	
2.593E-05	3.480E-03	25	P051	2 1 1 2 2	
2.593E-05	3.480E-03	25.00	P007	2 1 2 2 2	
1.445E-04	1.940E-02	ns	D001	0 0 0 0 2	
7.152E-05	9.600E-03	ns	H123	0 0 0 0 0	

2188. $C_{10}H_{14}$
Butylbenzene
1-Phenylbutane
n-Butylbenzene
RN: 68411-44-9 **MP** (°C)**:** –88
MW: 134.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.745E+00	ns	H307	0 0 0 0 0	

2189. $C_{10}H_{14}$
n-Butylbenzene
1-Phenylbutane
Butylbenzene
RN: 104-51-8 **MP** (°C)**:** –88.5
MW: 134.22 **BP** (°C)**:** 183.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.940E-05	1.334E-02	7	O312	2 2 0 2 2	
9.670E-05	1.298E-02	10	O312	2 2 0 2 2	
9.790E-05	1.314E-02	12.5	O312	2 2 0 2 2	
9.660E-05	1.297E-02	15	O312	2 2 0 2 2	
9.790E-05	1.314E-02	17.5	O312	2 2 0 2 2	
9.909E-05	1.330E-02	20	B356	0 0 0 0 0	
1.018E-04	1.366E-02	20	O312	2 2 0 2 2	
9.387E-06	1.260E-03	25	A002	1 2 1 1 2	*sic*
3.700E-04	4.966E-02	25	K001	1 0 2 1 2	
1.320E-04	1.772E-02	25	M124	2 1 2 2 2	
1.030E-04	1.382E-02	25	M342	1 0 1 1 2	
1.025E-04	1.376E-02	25	O312	2 2 0 2 2	
8.791E-05	1.180E-02	25	S005	2 2 2 2 2	
3.725E-04	5.000E-02	25	S012	2 0 2 2 0	
8.791E-05	1.180E-02	25	S191	1 2 2 2 2	
8.791E-05	1.180E-02	25	S358	2 1 2 2 2	
1.030E-04	1.382E-02	25	W300	2 2 2 2 2	
1.244E-04	1.670E-02	29.99	C350	0 0 0 0 0	
1.086E-04	1.458E-02	30	O312	2 2 0 2 2	
1.147E-04	1.540E-02	35	O312	2 2 0 2 2	
1.328E-04	1.782E-02	39.99	C350	0 0 0 0 0	
1.234E-04	1.656E-02	40	O312	2 2 0 2 2	
1.411E-04	1.894E-02	45	O312	2 2 0 2 2	
1.517E-04	2.036E-02	49.99	C350	0 0 0 0 0	
2.006E-04	2.692E-02	59.99	C350	0 0 0 0 0	
2.389E-04	3.206E-02	69.99	C350	0 0 0 0 0	
3.555E-04	4.772E-02	79.99	C350	0 0 0 0 0	
4.555E-04	6.114E-02	89.99	C350	0 0 0 0 0	
6.222E-04	8.351E-02	99.99	C350	0 0 0 0 0	
9.387E-05	1.260E-02	ns	H123	0 0 0 0 0	

2190. $C_{10}H_{14}$
p-Cymene
1-Methyl-4-isopropylbenzene
4-Cymene
Dolcymine
RN: 99-87-6 **MP** (°C)**:** –68
MW: 134.22 **BP** (°C)**:** 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-03	3.998E-01	25	B019	1 0 1 2 0	*sic*
1.740E-04	2.335E-02	25	B173	2 0 2 2 2	*sic*

2191. $C_{10}H_{14}$
sec-Butylbenzene
1-Methylpropylbenzene
RN: 135-98-8 **MP** (°C)**:** –82.7
MW: 134.22 **BP** (°C)**:** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.302E-03	3.090E-01	25	A002	1 2 1 1 2	*sic*
7.525E-05	1.010E-02	25	K119	1 0 0 0 2	
1.311E-04	1.760E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
1.311E-04	1.760E-02	25	S358	2 1 2 2 2	

2192. $C_{10}H_{14}$
tert-Butylbenzene
1,1-Dimethylethylbenzene
t-Butylbenzene
RN: 98-06-6 **MP** (°C)**:** –58
MW: 134.22 **BP** (°C)**:** 168.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-04	3.400E-02	25	A002	1 2 1 1 1	
2.198E-04	2.950E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
2.198E-04	2.950E-02	25	S358	2 1 2 2 2	

2193. $C_{10}H_{14}$
1,2-Diethylbenzene
o-Diethylbenzene
RN: 135-01-3 **MP** (°C)**:** –31
MW: 134.22 **BP** (°C)**:** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	7.114E-02	10	B149	2 1 1 2 1	
5.300E-04	7.114E-02	20	B149	2 1 1 2 1	

2194. $C_{10}H_{14}$
1,4-Diethylbenzene
p-Diethylbenzene
RN: 105-05-5 **MP** (°C)**:** –43
MW: 134.22 **BP** (°C)**:** 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	2.483E-02	10	B149	2 1 1 2 2	
1.850E-04	2.483E-02	20	B149	2 1 1 2 2	

2195. $C_{10}H_{14}Cl_2NO_2PS$
DMPA
Isopropylphosphoramidothioate
O-(2,4-Dichlorophenyl)-*O*-methyl
Phosphoramidothioic acid, isopropyl-*o*-(2,4-dichlorophenyl)-*o*-methyl ester
RN: 299-85-4 **MP** (°C)**:** 51.4
MW: 314.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.595E-05	5.010E-03	25	B185	0 0 0 0 0	
1.591E-05	5.000E-03	25	B200	1 0 0 0 0	
1.591E-05	5.000E-03	ns	M061	0 0 0 0 0	

2196. $C_{10}H_{14}Cl_6N_4O_2$
Triforine
N,N′-[1,4-Piperazinediylbis(2,2,2-trichloroethylidene)] bisformamide
Funginex
Denarin
Biformylchlorazin
Saprol
RN: 26644-46-2 **MP** (°C)**:** 155
MW: 434.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.38E-05	~6.00E-03	rt	D303	0 0 0 0 0	
6.437E-05	2.800E-02	rt	M161	0 0 0 0 0	

2197. $C_{10}H_{14}NO_5PS$
Parathion
O,O-Diethyl *O*-*p*-nitrophenyl phosphorothioate
Foliclal
Rhodiatox
Alkron
Fosferno
RN: 56-38-2 **MP** (°C)**:** 6
MW: 291.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
4.257E-05	1.240E-02	20	B169	2 1 1 1 1	
8.318E-05	2.423E-02	20	B179	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
2.245E-05	6.540E-03	24	F179	2 2 2 2 2	
8.240E-05	2.400E-02	25	M161	1 0 0 0 1	

(*continued*)

2197. $C_{10}H_{14}NO_5PS$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
4.086E-05	1.190E-02	ns	F071	0 1 2 1 2	
8.240E-05	2.400E-02	ns	M061	0 0 0 0 1	
6.867E-05	2.000E-02	ns	M110	0 0 0 0 0	EFG
8.240E-05	2.400E-02	ns	M344	0 0 0 0 1	

2198. $C_{10}H_{14}NO_6P$

Paraoxon
Diethyl *p*-nitrophenyl phosphate
Fosfacol
Eticol
Ethyl paraoxon
Miotisal

RN: 311-45-5 **MP** (°C)**:**
MW: 275.20 **BP** (°C)**:** 169–170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-02	3.627E+00	20	B169	2 0 1 1 2	
3.634E-03	1.000E+00	20	F300	1 0 0 0 0	

2199. $C_{10}H_{14}N_2O$

N-(Dimethylaminomethyl)benzamide
Benzamide, *N*-[(dimethylamino)methyl]-

RN: 59917-58-7 **MP** (°C)**:**
MW: 178.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	4.634E+02	22	J037	0 0 0 0 0	

2200. $C_{10}H_{14}N_2O$

N-(Ethylaminomethyl)benzamide
Benzamide, *N*-[(ethylamino)methyl]-

RN: 73239-20-0 **MP** (°C)**:**
MW: 178.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-02	1.301E+01	22	J037	0 0 0 0 0	

2201. $C_{10}H_{14}N_2O_2$
m-N,N-Dimethylaminophenyl *N*-methylcarbamate
1,3-*N,N*-Dimethylaminophenyl *N*-methylcarbamate
RN: 2631-39-2 **MP** (°C)**:** 86
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.604E-03	7.000E-01	30	D089	2 2 0 0 0	

2202. $C_{10}H_{14}N_2O_3$
5-Methyl-5-(3-methylbut-2-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(3-methyl-2-butenyl)
5-Methyl-5-(3-methylbut-2-enyl)barbiturate
RN: 66843-01-4 **MP** (°C)**:**
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.503E-03	5.262E-01	25	P350	0 0 0 0 0	intrinsic

2203. $C_{10}H_{14}N_2O_3$
2,4-Diazaspiro[5.6]dodecane-1,3,5-trione
Cycloheptane-spirobarbiturate
RN: 143288-61-3 **MP** (°C)**:**
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.790E-04	1.427E-01	25	P350	0 0 0 0 0	intrinsic

2204. $C_{10}H_{14}N_2O_3$
5-Isopropyl-5-allylbarbituric acid
Aprobarbital
5-(1-Methylethyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-isopropylbarbituric acid
Aprobarbitone
RN: 77-02-1 **MP** (°C)**:** 141
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.617E-02	3.400E+00	20	J030	1 2 2 2 2	
1.960E-02	4.121E+00	25	P350	0 0 0 0 0	intrinsic
1.940E-02	4.079E+00	25	V033	2 0 1 1 2	
1.940E-02	4.079E+00	25.00	T303	1 0 0 0 2	
2.600E-02	5.466E+00	35.00	T303	1 0 0 0 2	
2.664E-02	5.600E+00	37	J030	1 2 2 2 2	
3.340E-02	7.022E+00	45.00	T303	1 0 0 0 2	
1.912E-02	4.020E+00	ns	T003	0 0 0 0 2	

2205. $C_{10}H_{14}N_2O_5$
Thymidine
(1-[2-Deoxy-β-D-ribofuranosyl]-5-methyluracil)
Thyminedeoxyriboside
2′-deoxy-5-methyl
Thymine-2-desoxyriboside
Uridine
RN: 50-89-5 **MP** (°C)**:** 187–189
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	6.589E+00	19.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.96	T418	0 0 0 0 0	
2.780E-02	6.734E+00	24.99	T418	0 0 0 0 0	
3.040E-02	7.364E+00	24.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.99	T418	0 0 0 0 0	
2.870E-02	6.952E+00	24.99	T418	0 0 0 0 0	
2.200E-01	5.329E+01	24.99	T418	0 0 0 0 0	
2.710E-02	6.565E+00	25.49	T418	0 0 0 0 0	

2206. $C_{10}H_{14}N_2S$
Methiuron
N,N-Dimethyl-*N′*-3-methylphenylthiourea
RN: 21540-35-2 **MP** (°C)**:** 145
MW: 194.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-03	4.000E-01	ns	M061	0 0 0 0 2	

2207. $C_{10}H_{14}N_4O_2$
7-Propyl theophylline
3,7-Dimethyl-7-propyl-xanthine
RN: 27760-74-3 **MP** (°C)**:**
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E+00	2.320E+02	30	B042	1 2 1 1 2	
1.040E+00	2.311E+02	30	G021	1 0 0 0 2	

2208. $C_{10}H_{14}N_4O_2$
1-Propyl theobromine
3,7-Dimethyl-1-propyl-xanthine
RN: 204443-29-8 **MP** (°C)**:** 99
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.190E-02	1.376E+01	30	B042	1 2 1 1 2	

2209. $C_{10}H_{14}N_4O_3$
Ethoxycaffeine
1,3,7-Trimethyl-2,6-dioxo-8-ethoxypurine
RN: 577-66-2 **MP** (°C)**:** 143
MW: 238.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-02	2.991E+00	19	A072	1 2 1 0 1	

2210. $C_{10}H_{14}N_4O_4$
Dyphylline
7-(2,3-Dihydroxypropyl)theophylline
Lufyllin-EPG
Neothylline
Airet
RN: 479-18-5 **MP** (°C)**:** 158
MW: 254.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-01	1.700E+02	37	F076	2 0 2 2 1	

2211. $C_{10}H_{14}N_5O_7P$
2′-Adenylic acid
2′-Adenylsaeure
RN: 130-49-4 **MP** (°C)**:**
MW: 347.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2212. $C_{10}H_{14}N_5O_7P$
3′-Adenylic acid
3′-Adenylsaeure
RN: 84-21-9 **MP** (°C)**:** 197
MW: 347.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2213. $C_{10}H_{14}O$

L-Carvone
r-(–)-*p*-Mentha-6,8-dien-2-one
1-Methyl-4-isopropenyl-6-cyclohexen-2-one
p-Mentha-6,8-dien-2-one
RN: 6485-40-1 **MP** (°C)**:** <25
MW: 150.22 **BP** (°C)**:** 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.654E-03	1.300E+00	18	F300	1 0 0 0 1	
8.654E-03	1.300E+00	25	A049	1 0 0 0 1	
1.020E-02	1.532E+00	25	A401	1 0 2 2 0	
1.100E-02	1.652E+00	25	D407	1 0 2 2 2	
1.100E-02	1.652E+00	37	E028	1 0 1 1 2	

2214. $C_{10}H_{14}O$

l-Perillaldehyde
4-Isopropenyl-1-cyclohexene-1-carboxaldehyde
para-Mentha-1,8-dien-7-al
L-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde
L(–)-Perillaldehyde
(*S*)-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde
RN: 18031-40-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	6.309E-01	25	A401	1 0 2 2 0	

2215. $C_{10}H_{14}O$

p-*n*-Butylphenol
4-*n*-Butylphenol
RN: 1638-22-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.038E-03	4.563E-01	20	R087	0 0 0 0 0	0.15M NaCl
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2216. $C_{10}H_{14}O$

o-*n*-Butylphenol
2-*n*-Butylphenol
RN: 28805-86-9 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2217. $C_{10}H_{14}O$
p-tert-Butylphenol
4-*t*-Butylphenol
RN: 98-54-4 **MP** (°C)**:** 99.5
MW: 150.22 **BP** (°C)**:** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.327E-03	6.500E-01	22.5	G301	0 0 0 0 0	
3.327E-03	4.998E-01	25	L021	1 0 0 0 0	
3.861E-03	5.800E-01	25	M127	1 0 0 0 1	
4.427E-03	6.650E-01	25	P004	0 0 0 0 0	
5.076E-03	7.625E-01	30	P004	0 0 0 0 0	
5.785E-03	8.690E-01	35	P004	0 0 0 0 0	
6.534E-03	9.815E-01	40	P004	0 0 0 0 0	
4.266E-03	6.408E-01	ns	R427	0 0 0 0 0	

2218. $C_{10}H_{14}O$
Thymol
6-Isopropyl-*m*-cresol
3-Hydroxy-*p*-cymene
5-Methyl-2-isopropyl-1-phenol
2-Isopropyl-5-methyl phenol
5-Methyl-2-(1-methylethyl)phenol
RN: 89-83-8 **MP** (°C)**:** 48–51
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.991E-03	9.000E-01	20	F300	1 0 0 0 0	
6.000E-03	9.013E-01	25	D407	1 0 2 2 2	
5.700E-03	8.563E-01	25	F044	1 0 0 0 1	
6.046E-03	9.083E-01	25	L021	1 0 0 0 0	
6.650E-03	9.990E-01	25	R041	0 0 0 0 0	
5.990E-02	8.998E+00	37	E028	1 0 1 1 2	*sic*
8.654E-03	1.300E+00	37	F300	1 0 0 0 1	
6.166E-03	9.263E-01	ns	R427	0 0 0 0 0	

2219. $C_{10}H_{14}O$
Carvacrol
2-Methyl-5-isopropylphenol
RN: 499-75-2 **MP** (°C)**:** 3
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-03	9.990E-01	25	L021	1 0 0 0 0	
8.321E-03	1.250E+00	25	M127	1 0 0 0 2	

2220. $C_{10}H_{14}O$
4-*sec*-Butylphenol
p-*sec*-Butylphenol
RN: 99-71-8 **MP** (°C)**:**
MW: 150.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-03	9.600E-01	25	M127	1 0 0 0 1	

2221. $C_{10}H_{14}O_2$
3-Butoxyphenol
m-Butoxy phenol
Phenol, 3-butoxy-
RN: 18979-72-1 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.240E-03	1.370E+00	30	B315	0 0 0 0 0	

2222. $C_{10}H_{14}O_2$
p-Diethoxybenzene
4-Diethoxybenzene
RN: 122-95-2 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.560E-04	7.580E-02	25	C316	0 0 0 0 0	0.1M NaCl

2223. $C_{10}H_{14}O_2$
o-Butoxyphenol
2-Butoxyphenol
RN: 39075-90-6 **MP** (°C)**:**
MW: 166.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-03	6.516E-01	24.99	B353	0 0 0 0 0	

2224. $C_{10}H_{14}O_8$

1,1,2,2-Ethanetetrol, tetraacetate
Glyoxal-tetraacetat
Glyoxal tetraacetate
RN: 59602-16-3 **MP** (°C)**:**
MW: 262.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-05	8.000E-03	25	F300	1 0 0 0 1	

2225. $C_{10}H_{15}N$

Diethylaniline
2,6-Diethylaniline
RN: 579-66-8 **MP** (°C)**:** –38
MW: 149.24 **BP** (°C)**:** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.489E-03	6.700E-01	26.70	L095	2 2 1 1 2	
4.467E-03	6.666E-01	ns	S460	0 0 0 0 0	

2226. $C_{10}H_{15}NO$

Ethyl phenyl ethanolamine
2-(*N*-Ethylanilino)ethanol
N-Phenyl-*N*-ethylethanolamine
RN: 92-50-2 **MP** (°C)**:**
MW: 165.24 **BP** (°C)**:** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-02	4.975E+00	20	M062	1 0 0 0 1	

2227. $C_{10}H_{15}NO$

Ephedrine
L-Erythro-2-(methylamino)-1-phenylpropan-1-ol
(1*R*,2*S*)-(–)-Ephedrine
L-α-(1-Methylaminoethyl)benzyl alcohol
RN: 299-42-3 **MP** (°C)**:** 38–39
MW: 165.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.882E-01	4.762E+01	25	D004	0 0 0 0 0	
3.442E-01	5.688E+01	25	L338	1 0 1 1 2	
3.850E-01	6.362E+01	30	L069	1 0 1 1 0	EFG
1.160E+00	1.917E+02	ns	F007	0 0 0 0 2	

2228. $C_{10}H_{15}NO$
(+)-Pseudoephedrine
(+)-Pseudoephedrin
RN: 90-82-4 **MP** (°C)**:** 118
MW: 165.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.03E-03	<5.00E-01	rt	B435	0 0 0 0 0	

2229. $C_{10}H_{15}NO_2$
N-Phenyldiethanolamine
Phenyl diethanolamine
N,N-di(Hydroxyethyl)aniline
2,2′-(Phenylimino)diethanol
PDEA
RN: 120-07-0 **MP** (°C)**:** 57
MW: 181.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-01	3.232E+01	20	M062	1 0 0 0 2	

2230. $C_{10}H_{15}N_5O_5$
Arabinosyladenine
9-β-D-Arabino furanosyl adenine
Vidarabine
β-D-Arabinosyladenine
Spongoadenosine
RN: 24356-66-9 **MP** (°C)**:** 208
MW: 285.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	5.135E-01	ns	R030	0 0 0 0 0	

2231. $C_{10}H_{15}OPS_2$
Fonofos
Ethyl *S*-phenyl ethylphosphonothiolthionate
Diphonate
Dyfonate®
Stauffer N-2790
RN: 944-22-9 **MP** (°C)**:**
MW: 246.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-05	1.570E-02	20	B169	2 1 1 1 2	
6.089E-05	1.500E-02	ns	M110	0 0 0 0 0	EFG

(*continued*)

2231. $C_{10}H_{15}OPS_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.272E-05	1.299E-02	ns	S460	0 0 0 0 0	
6.374E-05	1.570E-02	ns	V414	0 0 0 0 0	

2232. $C_{10}H_{15}O_3PS_2$

Fenthion
4-Methylmercapto-3-methylphenyl dimethyl thiophosphate
Mercaptofos
Thiophos
Baycid
Entex

RN: 55-38-9 **MP** (°C)**:** 7.5
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-05	6.400E-03	10	B324	0 0 0 0 0	
2.300E-05	6.402E-03	10	B324	0 0 0 0 0	
2.698E-05	7.509E-03	20	B300	2 1 1 1 2	
3.244E-05	9.029E-03	20	B324	0 0 0 0 0	
3.341E-05	9.300E-03	20	B324	0 0 0 0 0	
1.940E-04	5.400E-02	20	M061	1 0 0 0 1	
4.074E-05	1.134E-02	30	B324	0 0 0 0 0	
4.060E-05	1.130E-02	30	B324	0 0 0 0 0	
1.976E-04	5.500E-02	rt	M161	0 0 0 0 0	

2233. $C_{10}H_{16}$

Myrcene
7-Methyl-3-methylene-1,6-octadiene
7-Methyl-3-methylene-1,6-octadiene
7-Methyl-3-methyleneocta-1,6-diene
7-Methyl-3-methylene-octadiene
β-Myrcene

RN: 123-35-3 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	4.087E-03	25	A401	1 0 2 2 0	
7.560E-05	1.030E-02	25	L450	0 0 0 0 0	

2234. $C_{10}H_{16}$
β-Pinene
(10)-Pinene
Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-
Nopinene
Pseudopinene
RN: 127-91-3 **MP** (°C)**:** –61
MW: 136.24 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	1.272E-02	24.99	T424	0 0 0 0 0	
8.808E-05	1.200E-02	25	L450	0 0 0 0 0	

2235. $C_{10}H_{16}$
D-Limonene
D-1,8-*p*-Menthadiene
(*R*)-1-Methyl-4-(1-methylethenyl)cyclohexene
(*R*)-(+)-Limonene
Hemo-sol
RN: 5989-27-5 **MP** (°C)**:** 95
MW: 136.24 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.080E-01	9.646E+01	0	M124	2 1 2 2 1	
7.670E-01	1.045E+02	5	M124	2 1 2 2 2	
6.973E-05	9.500E-03	25	L450	0 0 0 0 0	
1.011E-04	1.377E-02	25	M124	2 1 2 2 1	

2236. $C_{10}H_{16}$
Limonene
p-Mentha-1,8-diene
Cyclil decene
Acintene DP dipentene
RN: 138-86-3 **MP** (°C)**:** 73.97
MW: 136.24 **BP** (°C)**:** 175.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-05	4.332E-03	6	P430	0 0 0 0 0	
4.100E-05	5.586E-03	23.5	P430	0 0 0 0 0	
9.055E-05	1.234E-02	24.99	T424	0 0 0 0 0	
6.390E-05	8.706E-03	25	I019	1 0 1 2 2	
2.202E-04	3.000E-02	25	M350	1 0 1 1 1	

2237. $C_{10}H_{16}$
γ-Terpinene
1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene
1,4-*p*-Menthadiene
1-Isopropyl-4-methyl-1,4-cyclohexadiene
Moslene
Terpinene
RN: 99-85-4 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-05	6.090E-03	6	P430	0 0 0 0 0	
6.370E-05	8.678E-03	23.5	P430	0 0 0 0 0	

2238. $C_{10}H_{16}$
Terpinolene
1-Methyl-4-(1-methylethylidene)cyclohexene
1,4(8)-*p*-Menthadiene
1-Methyl-4-(1-methylethylidene)cyclohexene
Terpinolene 30/35
Terpinolene 90
RN: 586-62-9 **MP** (°C)**:**
MW: 136.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.670E-05	7.725E-03	6	P430	0 0 0 0 0	
6.960E-05	9.482E-03	23.5	P430	0 0 0 0 0	
5.000E-05	6.812E-03	25	A401	1 0 2 2 0	

2239. $C_{10}H_{16}$
α-Pinene
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene
Acitene A
Cyclic dexadiene
pin-2(3)-ene
2-Pinene
RN: 80-56-8 **MP** (°C)**:** –64
MW: 136.24 **BP** (°C)**:** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-05	2.275E-03	6	P430	0 0 0 0 0	
1.830E-05	2.493E-03	23.5	P430	0 0 0 0 0	
3.867E-05	5.268E-03	24.99	T424	0 0 0 0 0	
3.523E-05	4.800E-03	25	L450	0 0 0 0 0	

2240. $C_{10}H_{16}Cl_3NOS$
Triallate
S-(2,3,3-Trichloroallyl)diisopropylthiocarbamate
RN: 2303-17-5 **MP** (°C)**:** 29
MW: 304.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-05	4.000E-03	25	B200	1 0 0 1 0	
1.313E-05	4.000E-03	25	M161	1 0 0 0 0	
1.313E-05	4.000E-03	ns	F019	0 0 0 0 0	

2241. $C_{10}H_{16}NO_2S_2$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dithiolane
2-Cyclopentyl-4-methoxycarbamyl-1,3-dithiolane
RN: **MP** (°C)**:**
MW: 246.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.391E-02	rt	B174	0 0 1 0 0	

2242. $C_{10}H_{16}NO_3S$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-oxathiolane
RN: **MP** (°C)**:**
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-03	3.455E-01	rt	B174	0 0 1 0 1	

2243. $C_{10}H_{16}NO_4$
2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dioxolane
RN: **MP** (°C)**:**
MW: 214.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.785E+00	rt	B174	0 0 1 0 1	

2244. $C_{10}H_{16}N_2O_3$
5-Ethyl-5-(2-methylpropyl)barbituric acid
RN: 125-40-6 **MP** (°C)**:** 174.5
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.997E-03	8.483E-01	25	B065	1 2 1 1 1	

2245. $C_{10}H_{16}N_2O_3$
5,5-Dipropylbarbituric acid
5,5-Dipropylbarbitursaeure
Proponal
5,5-Dipropylbarbiturate
RN: 2217-08-5 **MP** (°C)**:** 146
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-03	6.000E-01	20	F300	1 0 0 0 0	
2.968E-03	6.300E-01	20	J030	1 2 2 2 1	
5.088E-03	1.080E+00	37	J030	1 2 2 2 2	
6.926E-02	1.470E+01	100	F300	1 0 0 0 2	

2246. $C_{10}H_{16}N_2O_3$
5,5-Diisopropylbarbituric acid
Barbituric acid, 5,5-diisopropyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-bis(1-methylethyl)
5,5-Di-i-propylbarbiturate
RN: 99167-69-8 **MP** (°C)**:**
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E-03	3.640E-01	25	P350	0 0 0 0 0	intrinsic

2247. $C_{10}H_{16}N_2O_3$
Butabarbital
Butethal
5-Ethyl-5-*n*-butylbarbituric acid
5-Butyl-5-ethylbarbituric acid
RN: 77-28-1 **MP** (°C)**:** 127
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.602E-02	3.400E+00	0	D089	0 0 0 0 2	form I
1.484E-02	3.150E+00	20	J030	1 2 2 2 2	
1.044E-02	2.215E+00	20	K078	1 0 2 1 2	
4.052E-03	8.600E-01	25	B011	2 0 0 1 0	
4.218E-03	8.954E-01	25	B065	1 1 1 1 1	
1.936E-02	4.110E+00	25	B065	1 1 1 1 1	
8.000E-03	1.698E+00	25	G003	1 1 1 1 1	pH 4.7
2.300E-02	4.882E+00	25	M310	2 2 2 2 2	
2.130E-02	4.521E+00	25	V033	2 0 1 1 2	
4.070E-03	8.639E-01	25	V033	2 0 1 1 2	
2.130E-02	4.521E+00	25.00	T303	1 0 0 0 2	
7.400E-03	1.571E+00	25.00	T303	1 0 0 0 1	

(*continued*)

2247. $C_{10}H_{16}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-02	4.139E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
9.900E-03	2.101E+00	35.00	T303	1 0 0 0 1	
2.430E-02	5.158E+00	35.00	T303	1 0 0 0 2	
2.299E-02	4.880E+00	37	J030	1 2 2 2 2	
3.090E-02	6.559E+00	45.00	T303	1 0 0 0 2	
1.370E-02	2.908E+00	45.00	T303	1 0 0 0 2	
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form II
1.602E-02	3.400E+00	amb	D092	0 2 2 1 2	0.1N HCl, form III, mp 124 C
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form I
9.362E-03	1.987E+00	ns	T003	0 0 0 0 2	
8.952E-03	1.900E+00	ns	T003	0 0 0 0 2	

2248. $C_{10}H_{16}N_2O_3S$

Biotin d
D-Biotin
Biotin

RN: 58-85-5 **MP** (°C)**:** 232
MW: 244.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.003E-04	2.200E-01	25	D041	1 0 0 0 1	
1.433E-03	3.500E-01	25	D315	0 0 0 0 0	
8.186E-04	2.000E-01	25	M054	1 0 0 0 0	

2249. $C_{10}H_{16}N_2O_4$

Methyl-2,2-diallylmalonurate
Methyl 2,2-diallylmalonurate

RN: 73632-82-3 **MP** (°C)**:** 84
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.552E+00	23	B152	1 2 1 1 1	pH 3.5

2250. $C_{10}H_{16}N_4O_2$

7-Butyl theophylline
1H-Purine-2,6-dione, 7-butyl-3,7-dihydro-1,3-dimethyl-
7-Butyl-1,3-dimethylxanthine

RN: 1021-65-4 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	3.499E+00	30	B042	1 2 1 1 2	
1.560E-02	3.499E+00	30	G021	1 0 0 0 2	

2251. $C_{10}H_{16}N_4O_2S$

3-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-4-hydroxy-1
2-Imidazolidinone, 3-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-4-hydroxy-1-methyl-
Buthidazole
Ravage
VEL 5026

RN: 55511-98-3 **MP** (°C)**:** 133.5
MW: 256.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.322E-02	3.388E+00	25	M161	1 0 0 0 1	

2252. $C_{10}H_{16}N_6S$

Cimetidine
2-Cyano-1-methyl-3-(2-(((5-methylimidazol-4-yl)methyl)thio)ethyl)guanidine
N″-Cyano-*N*-methyl-*N′*-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine
N″-Cyano-*N*-methyl-*N′*-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine
Sigmetadine
Peptol

RN: 51481-61-9 **MP** (°C)**:** 142
MW: 252.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	6.010E+00	22.5	B422	2 0 2 2 2	
3.685E-02	9.300E+00	25	A412	1 0 2 2 1	int
3.963E-03	1.000E+00	ns	K444	0 0 0 0 0	

2253. $C_{10}H_{16}O$

D-Fenchone
D-1,3,3-Trimethyl-2-norbornanone
Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1*S*)-
α-Fenchone
(+)-Fenchone

RN: 4695-62-9 **MP** (°C)**:** 6.1
MW: 152.24 **BP** (°C)**:** 193.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-02	1.996E+00	20	D052	1 1 0 0 0	
1.410E-02	2.147E+00	25	I019	1 0 1 2 2	
1.413E-02	2.150E+00	ns	S460	0 0 0 0 0	

2254. $C_{10}H_{16}O$
D-Camphor
D-Campher
Camphor
RN: 76-22-2 **MP** (°C)**:** 179.7
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	1.667E+00	15.50	L073	1 2 2 1 2	
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	
1.363E-02	2.076E+00	20	K078	1 0 2 1 2	
1.030E-02	1.568E+00	25	I019	1 0 1 2 2	
1.340E-02	2.040E+00	25	L338	1 0 1 1 2	
1.630E-02	2.481E+00	37	E028	1 0 1 1 2	
1.115E-02	1.697E+00	ns	F014	0 0 0 0 2	
1.023E-02	1.558E+00	ns	R427	0 0 0 0 0	

2255. $C_{10}H_{16}O$
Carvotan acetone
Carvotan-aceton
RN: 499-71-8 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.912E-03	9.000E-01	20	F300	1 0 0 0 0	

2256. $C_{10}H_{16}O$
Citral
trans-3,7-dimethyl-2,6-octadienal
Geranialdehyde
Neral
Geranial
Citral A
RN: 5392-40-5 **MP** (°C)**:** <10
MW: 152.24 **BP** (°C)**:** 92.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	5.785E-01	25	A401	1 0 2 2 0	
1.583E-03	2.410E-01	25	L450	0 0 0 0 0	
1.970E-03	2.999E-01	25	M350	1 0 1 1 1	
8.800E-03	1.340E+00	37	E028	1 0 1 1 1	
8.710E-03	1.326E+00	ns	S460	0 0 0 0 0	

2257. $C_{10}H_{16}O$
L-Dihydrocarvone
L-Dihydro-carvon
RN: 619-02-3 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:** 221

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	

2258. $C_{10}H_{16}O$
Neral
RN: 106-26-3 **MP** (°C)**:**
MW: 152.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.898E-03	2.890E-01	25	L450	0 0 0 0 0	

2259. $C_{10}H_{16}O_2$
3-Hydroxy-3-ethynyl-2,2,5,5-tetramethyltetrahydrofuran
3-Furanol, 3-ethynyltetrahydro-2,2,5,5-tetramethyl-
RN: 24270-82-4 **MP** (°C)**:**
MW: 168.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.165E-01	1.961E+01	rt	B066	0 2 0 0 0	

2260. $C_{10}H_{16}O_3$
cis-Pinonic acid
cis-3-Acetyl-2,2-dimethylcyclobutaneacetic acid
RN: 473-72-3 **MP** (°C)**:** 104–107
MW: 184.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.001E-02	3.686E+00	0	H430	0 0 0 0 0	
3.612E-02	6.655E+00	rt	H431	0 0 0 0 0	average

2261. $C_{10}H_{16}O_4$
L-Isocamphoric acid
L-Isocamphersaeure
RN: 5394-83-2 **MP** (°C)**:** 173
MW: 200.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.698E-02	3.400E+00	20	F300	1 0 0 0 1	

2262. $C_{10}H_{16}O_4$

D-Camphoric acid
D-Camphersaeure
RN: 124-83-4 **MP** (°C)**:**
MW: 200.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.796E-02	7.600E+00	25	F300	1 0 0 0 1	

2263. $C_{10}H_{16}O_5$

DL-Cineolic acid
DL-Cineolsaeure
RN: 473-18-7 **MP** (°C)**:** 208
MW: 216.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-02	1.400E+01	15	F300	1 0 0 0 1	
3.006E-01	6.500E+01	100	F300	1 0 0 0 1	

2264. $C_{10}H_{17}Cl_2NOS$

Diallate
DATC
S-(2,3-Dichloroallyl-*N,N*-diisopropylthiocarbamate
RN: 2303-16-4 **MP** (°C)**:** –10
MW: 270.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	4.000E-02	25	B185	0 0 0 0 0	
5.181E-05	1.400E-02	25	B200	1 0 0 1 1	
1.480E-04	4.000E-02	25	M061	1 0 0 0 1	
5.181E-05	1.400E-02	25	M161	1 0 0 0 1	
1.480E-04	4.000E-02	ns	F019	0 0 0 0 1	
1.480E-04	4.000E-02	rt	I314	0 0 0 0 0	

2265. $C_{10}H_{17}NO_2$

Methyprylon
Dimerin
3,3-Diethyl-5-methyl-2,4-piperidinedione
RN: 125-64-4 **MP** (°C)**:**
MW: 183.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.147E-01	7.600E+01	25	R027	0 0 0 0 0	

2266. $C_{10}H_{17}N_2O_4PS$
Etrimfos
Dimethyl *O*-(2-ethyl-4-ethoxy-pyrimidin-6-yl)thionophosphate
Ekamet G
Ekamet ULV
Etrimphos
RN: 38260-54-7 **MP** (°C)**:**
MW: 292.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.421E-02	1.000E+01	20	M161	1 0 0 0 1	
1.368E-04	3.998E-02	ns	S460	0 0 0 0 0	

2267. $C_{10}H_{17}N_3O_5$
Orotic acid choline
RN: **MP** (°C)**:** 102–104
MW: 259.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.697E+00	6.992E+02	25	N018	0 0 0 0 0	

2268. $C_{10}H_{17}N_3O_6S$
Glutathione
Glutathion
RN: 70-18-8 **MP** (°C)**:** 193.4
MW: 307.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.958E-01	9.090E+01	0	F300	1 0 0 0 2	

2269. $C_{10}H_{17}O_3P$
Diethyl phenyl phosphonate
Diethyl benzenephosphonate
Diethyl phenylphosphonate
RN: 1754-49-0 **MP** (°C)**:**
MW: 216.22 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.25E-04	<2.00E-01	25	B070	1 2 0 1 0	

2270. $C_{10}H_{18}$
2,2,5,5-Tetramethyl-3-hexyne
Di-*tert*-butylacetylene
Di-*tert*-butylethyne
RN: 17530-24-4 **MP** (°C)**:**
MW: 138.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-04	2.032E-02	25	H039	1 2 2 2 2	
7.700E-05	1.065E-02	35	H039	1 2 2 2 1	

2271. $C_{10}H_{18}$
Pinane
2,6,6-Trimethylbicyclo[3.1.1]heptane
2,7,7-Trimethylbicyclo[3.1.1]heptane
Dihydropinene
RN: 473-55-2 **MP** (°C)**:**
MW: 138.25 **BP** (°C)**:** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-05	1.576E-03	ns	S460	0 0 0 0 0	

2272. $C_{10}H_{18}$
Decalin
Decahydronaphthalene
RN: 91-17-8 **MP** (°C)**:** –31
MW: 138.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.45E-03	<2.00E-01	25	B019	1 0 1 2 0	
6.430E-06	8.890E-04	25	P051	2 1 1 2 2	
6.148E-06	8.500E-04	25	T423	0 0 0 0 0	
6.430E-06	8.890E-04	25.00	P007	2 1 2 2 2	
4.492E-05	6.210E-03	ns	H123	0 0 0 0 0	

2273. $C_{10}H_{18}$
cis-Decalin
cis-Decahydronaphthalene
cis-Bicyclo[4.4.0]decane
RN: 493-01-6 **MP** (°C)**:** –43.2
MW: 138.25 **BP** (°C)**:** 195.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.452E-02	8.920E+00	300	S355	1 1 1 2 0	EFG

2274. $C_{10}H_{18}ClN_5$
Ipazine
2-Chloro-4-diethylamino-6-isopropylamino-*s*-triazine
2-Chloro-4-isopropylamino-6-biethylamino-*s*-triazines
RN: 1912-25-0 **MP** (°C)**:**
MW: 243.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	4.000E-02	21	B192	0 0 0 0 1	
1.641E-04	4.000E-02	21	G099	2 0 0 1 0	
1.641E-04	4.000E-02	ns	B185	0 0 0 0 0	

2275. $C_{10}H_{18}N_2O_4$
Ethyl-2,2-diethylmalonurate
Ethyl 2,2-diethylmalnurate
RN: 73632-76-5 **MP** (°C)**:** 84.5
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-03	1.934E+00	23	B152	1 2 1 1 1	pH 3.5

2276. $C_{10}H_{18}N_2O_5$
Methoxymethyl-2,2-diethylmalonurate
Methoxymethyl 2,2-diethylmalonurate
RN: 73632-79-8 **MP** (°C)**:** 113
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.675E+00	23	B152	1 2 1 1 1	pH 3.5

2277. $C_{10}H_{18}N_6O_2$
1-(Sarcosino)-3,5-bis(dimethylamino)-*s*-triazine
*N*2-Carboxymethyl-*N*2,*N*4,*N*4,*N*6,*N*6-pentamethylmelamine
RN: 64124-17-0 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.360E-02	1.872E+01	25	B386	0 0 0 0 0	

2278. $C_{10}H_{18}O$
Borneol
endo-1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol
L-Borneol
RN: 507-70-0 **MP** (°C)**:** 206
MW: 154.25 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.512E-03	6.960E-01	15	M073	1 0 2 2 2	
4.784E-03	7.380E-01	25	M073	1 0 2 2 2	
4.786E-03	7.383E-01	ns	R427	0 0 0 0 0	

2279. $C_{10}H_{18}O$
D-Borneol
Borneocamphor
Sumatra camphor
endo-2-Bornanol
RN: 464-43-7 **MP** (°C)**:** 208
MW: 154.25 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-03	7.400E-01	25	F300	1 0 0 0 1	

2280. $C_{10}H_{18}O$
L-Menthone
trans-p-Menthan-3-one
p-Menthan-3-one
(–)-5-Methyl-2-(1-methylethyl)cyclohexanone
(–)-Menthone
RN: 14073-97-3 **MP** (°C)**:** –6
MW: 154.25 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.220E-03	4.967E-01	25	I019	1 0 1 2 2	

2281. $C_{10}H_{18}O$
Linalool
3,7-Dimethylocta-1,6-dien-3-ol
2,6-Dimethylocta-2,7-dien-6-ol
Linalol
3,7-Dimethyl-1,6-octadien-3-ol
RN: 78-70-6 **MP** (°C)**:** <25
MW: 154.25 **BP** (°C)**:** 195.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.507E-01	6	P430	0 0 0 0 0	
5.530E-03	8.530E-01	23.5	P430	0 0 0 0 0	
1.200E-02	1.851E+00	25	D407	1 0 2 2 2	
1.030E-02	1.589E+00	25	I019	1 0 1 2 2	
9.710E-03	1.498E+00	25	M350	1 0 1 1 1	
3.800E-02	5.862E+00	37	E028	1 0 1 1 2	

2282. $C_{10}H_{18}O$
Citronellal
D-Citronellal
(*R*)-(+)-citronellal
3,7-Dimethyl-6-octen-1-al
3,7-Dimethyl-6-octenal
Rhodinal
RN: 106-23-0 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	1.388E-01	25	A401	1 0 2 2 0	

2283. $C_{10}H_{18}O$
α-Terpineol
1-*p*-Menthen-8-ol
1-Methyl-4-isopropyl-1-cyclohexen-8-ol
2-(4-Methyl-3-cyclohexenyl)-2-propanol
p-Menth-1-en-8-ol
α,α,4-Trimethyl-3-cyclohexene-1-methanol
RN: 98-55-5 **MP** (°C)**:** 34.5
MW: 154.25 **BP** (°C)**:** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.202E-03	3.397E-01	6	P430	0 0 0 0 0	
4.600E-03	7.096E-01	23.5	P430	0 0 0 0 0	
1.620E-02	2.499E+00	25	A401	1 0 2 2 0	

2284. $C_{10}H_{18}O$
Nerol
Allerol
cis-3,7-Dimethyl-2,6-octadien-1-ol
Neraniol
Nerosol
Vernol
RN: 106-25-2 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	1.311E+00	25	A401	1 0 2 2 0	

2285. $C_{10}H_{18}O$
Geraniol
2,6-Dimethyl-2,6-octadien-8-ol
2,6-Dimethyl-*trans*-2,6-octadien-8-ol
2-*trans*-3,7-Dimethyl-2,6-octadiene-1-ol
3,7-Dimethyl-*trans*-2,6-octadien-1-ol
(E)-3,7-Dimethyl-2,6-octadien-1-ol
RN: 106-24-1 **MP** (°C)**:** 15
MW: 154.25 **BP** (°C)**:** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	7.713E-01	25	A401	1 0 2 2 0	

2286. $C_{10}H_{18}O$
Menthone
5-Methyl-2-(1-methylethyl)cyclohexanone
DL-Menthone
RN: 10458-14-7 **MP** (°C)**:** –6
MW: 154.25 **BP** (°C)**:** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.085E-01	25	A401	1 0 2 2 0	

2287. $C_{10}H_{18}O$
Plinol
RN: 72402-00-7 **MP** (°C)**:**
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.281E-03	8.146E-01	6	P430	0 0 0 0 0	
9.610E-03	1.482E+00	23.5	P430	0 0 0 0 0	

2288. $C_{10}H_{18}O$
1,8-Cineole
Eucalyptol
Cineol
Cineole
RN: 470-82-6 **MP** (°C)**:** 36.5
MW: 154.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.123E-02	6.359E+00	1.5	E036	1 0 1 1 1	
4.187E-02	6.458E+00	4.0	B352	0 0 0 0 0	
3.674E-02	5.668E+00	7.5	E036	1 0 1 1 1	
3.482E-02	5.371E+00	10	E036	1 0 1 1 1	
3.610E-02	5.569E+00	10.0	B352	0 0 0 0 0	
1.297E-02	2.000E+00	15	F300	1 0 0 0 1	
3.097E-02	4.777E+00	15.0	B352	0 0 0 0 0	
2.261E-02	3.488E+00	21	E036	1 0 1 1 1	
2.454E-02	3.786E+00	21.0	B352	0 0 0 0 0	
2.010E-02	3.100E+00	25	A049	1 0 0 0 1	
2.197E-02	3.388E+00	25	B423	1 1 1 2 1	
1.746E-02	2.693E+00	30.0	B352	0 0 0 0 0	
1.552E-02	2.394E+00	35.0	B352	0 0 0 0 0	
9.100E-03	1.404E+00	37	E028	1 0 1 1 1	
1.359E-02	2.096E+00	40	E036	1 0 1 1 1	
1.423E-02	2.195E+00	40.0	B352	0 0 0 0 0	
1.294E-02	1.996E+00	45.0	B352	0 0 0 0 0	
1.229E-02	1.896E+00	50	E036	1 0 1 1 1	
1.100E-02	1.697E+00	50.0	B352	0 0 0 0 0	

2289. $C_{10}H_{18}O_2$
2,4-Decadione
Acetylmethyl hexyl ketone
RN: 13329-78-7 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.427E-01	25	M078	2 0 1 0 1	

2290. $C_{10}H_{18}O_2$
3-Pentyl-2,4-pentadione
3-Amyl-2,4-pentanedione
RN: 27970-50-9 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	2.401E+00	25	M078	2 0 1 0 2	

2291. $C_{10}H_{18}O_2$
Sobrerol
Pinolhydrat
RN: 498-71-5 **MP** (°C)**:** 130
MW: 170.25 **BP** (°C)**:** 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-01	3.200E+01	15	F300	1 0 0 0 1	
1.938E-01	3.300E+01	ns	L335	0 0 0 0 2	

2292. $C_{10}H_{18}O_2$
D-Campholic acid
D-Campholsaeure
RN: 464-88-0 **MP** (°C)**:**
MW: 170.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.398E-04	1.600E-01	19	F300	1 0 0 0 1	

2293. $C_{10}H_{18}O_3$
2,2,5,5-Tetramethyl-tetrahydro-3-hydroxy-3-furanyl methyl ketone
Ketone, methyl tetrahydro-3-hydroxy-2,2,5,5-tetramethyl-3-furyl
RN: 24282-51-7 **MP** (°C)**:**
MW: 186.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2294. $C_{10}H_{18}O_4$
Sebacic acid
Sebacinsaeure
RN: 111-20-6 **MP** (°C)**:** 134.5
MW: 202.25 **BP** (°C)**:** 294.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-04	4.000E-02	0	F300	1 0 0 0 0	
1.978E-04	4.000E-02	0	L041	1 0 0 1 0	
4.944E-03	1.000E+00	20	F300	1 0 0 0 1	
4.944E-03	1.000E+00	20	L041	1 0 0 1 1	
9.889E-03	2.000E+00	21	B040	1 0 1 1 1	*sic*
7.911E-03	1.600E+00	35	L041	1 0 0 1 1	
1.088E-02	2.200E+00	50	L041	1 0 0 1 1	
2.077E-02	4.200E+00	65	F300	1 0 0 0 1	
2.077E-02	4.200E+00	65	L041	1 0 0 1 1	
8.898E-04	1.800E-01	ns	F014	0 0 0 0 1	

2295. $C_{10}H_{18}O_4$
Amyl α-acetoxypropionate
Hydracrylic acid, pentyl ester, acetate
RN: 20473-77-2 **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.461E-03	7.000E-01	25	R006	2 2 0 1 1	

2296. $C_{10}H_{18}O_4$
Ethylene glycol dibutyrate
Ethylene glycol di-*N*-butyrate
RN: 105-72-6 **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-03	1.663E+00	25	F064	1 0 0 0 2	
2.471E-03	4.998E-01	ns	F014	0 0 0 0 1	

2297. $C_{10}H_{18}O_4$
Diethoxyethyl adipate
Diethyl adipate
RN: 141-28-6 **MP** (°C)**:** –18
MW: 202.25 **BP** (°C)**:** 251

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.965E-03	5.996E-01	ns	F014	0 0 0 0 1	
1.223E-02	2.474E+00	ns	F014	0 0 0 0 2	

2298. $C_{10}H_{18}O_4$
Dimethyl cyclohexyl oxalate
RN: **MP** (°C)**:**
MW: 202.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.89E-06	<2.00E-03	15	H069	1 0 1 1 0	

2299. $C_{10}H_{18}O_5$
Diethylene glycol dipropionate
Ethanol, 2,2′-oxybis-, dipropanoate
RN: 6942-59-2 **MP** (°C)**:**
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.592E-01	3.475E+01	ns	F014	0 0 0 0 2	

2300. $C_{10}H_{18}O_5$
Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, butyl ester
Propanoic acid, 2-[(amoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 218.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.290E-03	4.998E-01	25	R007	0 0 0 0 0	
3.205E-03	6.995E-01	25	R007	0 0 0 0 0	

2301. $C_{10}H_{19}NO_2S$
4-Thiazolidinecarboxylic acid, 2-hexyl-
Thiazolidine-4-carboxylic acid, 2-hexyl-
RN: 14347-74-1 **MP** (°C)**:**
MW: 217.33 **BP** (°C)**:** 378.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.085E-01	21	B414	1 0 0 1 1	partial decomposition

2302. $C_{10}H_{19}NO_3$
Ethylpropylaceturethane
RN: **MP** (°C)**:**
MW: 201.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.088E-03	1.427E+00	c	O021	0 2 0 0 0	

2303. $C_{10}H_{19}NO_3$
Oenanthylylurethane
RN: **MP** (°C)**:**
MW: 201.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.043E-03	2.100E-01	ns	O021	0 0 0 0 0	

2304. $C_{10}H_{19}NO_4S$
2-Amino-5-naphthol-1-sulfonic acid
RN: **MP** (°C)**:**
MW: 249.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.503E-03	2.120E+00	c	B125	1 2 0 0 2	

2305. $C_{10}H_{19}N_2O_4PS$

Cyanthoate
Phosphorothioic acid, *S*-(2-((1-cyano-1-methylethyl)amino)-2-oxoethyl) *O,O*-diethyl ester
Tartran
RN: 3734-95-0 **MP** (°C)**:**
MW: 294.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	7.000E+01	20	M161	1 0 0 0 1	

2306. $C_{10}H_{19}N_5O$

Prometone
2-Methoxy-4,6-*bis*-isopropylamino-*s*-triazine
Pramitol
Primatol O
Prometon
2-Methoxy-4,6-*bis*-(isopropyl-amino)-*s*-triazine
RN: 1610-18-0 **MP** (°C)**:** 91.5
MW: 225.30 **BP** (°C)**:** 91–92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.330E-03	7.502E-01	20	B200	1 0 0 0 2	
2.752E-03	6.200E-01	20	F311	1 2 2 2 1	
3.329E-03	7.500E-01	20	M161	1 0 0 0 2	
3.329E-03	7.500E-01	21	B192	0 0 0 0 2	
1.554E-02	3.500E+00	21	G099	2 0 0 1 0	
3.329E-03	7.500E-01	21	G099	2 0 0 1 0	
4.680E-03	1.054E+00	50	G001	1 0 1 1 2	
3.548E-03	7.994E-01	ns	B100	0 0 0 0 0	
3.329E-03	7.500E-01	ns	B185	0 0 0 0 0	
3.329E-03	7.500E-01	ns	C101	0 0 0 0 1	
3.329E-03	7.500E-01	ns	G041	0 0 0 0 2	
3.329E-03	7.500E-01	ns	H112	0 0 0 0 2	
3.329E-03	7.500E-01	ns	J033	0 0 0 0 0	

2307. $C_{10}H_{19}N_5O$

Terebumeton
1,3,5-Triazine-2,4-diamine, *N*-(1,1-dimethylethyl)-*N′*-ethyl-6-methoxy-
2-Methoxy-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Karagard
4-(Ethylamino)-2-methoxy-6-(*tert*-butylamino)-*s*-triazine
Caragard
RN: 33693-04-8 **MP** (°C)**:** 123.5
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.770E-04	1.300E-01	20	M161	1 0 0 0 2	

2308. $C_{10}H_{19}N_5O$
2-Methoxy-4-ethylamino-6-diethylamino-*s*-triazine
G 31432
RN: 13532-26-8 **MP** (°C)**:**
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-04	4.000E-02	20	J033	0 0 0 0 0	

2309. $C_{10}H_{19}N_5O$
Secbumeton
2-*sec*-Butylamino-4-ethylamino-6-methoxy-*s*-triazine
GS-14254
RN: 26259-45-0 **MP** (°C)**:** 86
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.930E-03	6.601E-01	1	G091	1 0 1 2 2	pH 6.0
3.250E-03	7.322E-01	8	G091	1 0 1 2 2	pH 6.0
2.750E-03	6.196E-01	20	B200	1 0 0 0 2	
2.663E-03	6.000E-01	20	F311	1 2 2 2 1	
3.070E-03	6.917E-01	20	G091	1 0 1 2 2	pH 6.0
2.752E-03	6.200E-01	20	M161	1 0 0 0 2	
3.300E-03	7.435E-01	29	G091	1 0 1 2 2	pH 6.0

2310. $C_{10}H_{19}N_5OS$
Hydroxyprometryne
1,3,5-Triazin-2(1H)-one, 4,6-bis[(1-methylethyl)amino]-
bis(Isopropylamino)hydroxy-*s*-triazine
GS 11526
RN: 7374-53-0 **MP** (°C)**:**
MW: 257.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.029E-01	2	B193	1 2 0 0 0	

2311. $C_{10}H_{19}N_5S$
Terbutryn
2-Methylthio-4-ethylamino-6-*tert*-butylamino-*s*-triazine
Terbutryne
N-(1,1-Dimethylethyl)-*N′*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Terbutrex
RN: 886-50-0 **MP** (°C)**:** 104
MW: 241.36 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	2.631E-02	1	G091	1 0 1 2 2	pH 6.0
1.100E-04	2.655E-02	8	G091	1 0 1 2 2	pH 6.0
2.400E-04	5.793E-02	20	B200	1 0 0 0 1	
1.036E-04	2.500E-02	20	E048	1 2 1 1 1	
1.036E-04	2.500E-02	20	F311	1 2 2 2 1	
1.460E-04	3.524E-02	20	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	20	M161	1 0 0 0 1	
1.660E-04	4.007E-02	29	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	ns	J033	0 0 0 0 0	

2312. $C_{10}H_{19}N_5S$
Prometryne
N,N′-bis(1-Methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine
Caparol
Primatol Q
Gesagard
Caparol 80W
RN: 7287-19-6 **MP** (°C)**:** 118
MW: 241.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.793E-02	2	B193	1 2 0 0 0	
2.000E-04	4.827E-02	20	B200	1 0 0 0 0	
1.657E-04	4.000E-02	20	F311	1 2 2 2 1	
1.988E-03	4.798E-01	20	M061	1 0 0 0 1	
1.989E-04	4.800E-02	20	M161	1 0 0 0 1	
1.989E-04	4.800E-02	24	C105	2 1 2 2 2	
4.200E-04	1.014E-01	50	G001	1 0 1 1 2	
1.989E-04	4.800E-02	ns	C101	0 0 0 0 1	
1.989E-04	4.800E-02	ns	H112	0 0 0 0 1	
1.989E-04	4.800E-02	ns	J033	0 0 0 0 0	

2313. $C_{10}H_{19}N_5S$
s-Triazole, 2,4-bis(isopropylamine)-6-methylmercapto-
RN: **MP** (°C)**:**
MW: 241.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E-04	4.800E-02	20	B185	0 0 0 0 0	

2314. $C_{10}H_{19}O_6PS_2$
Malathion
Dicarboethoxyethyl *O,O*-dimethyl phosphorodithioate
Carbofos
Cythion
Mercaptothion
Phosphothion
RN: 121-75-5 **MP** (°C)**:** 3
MW: 330.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.267E-04	1.410E-01	10	B324	0 0 0 0 0	
4.268E-04	1.410E-01	10	B324	0 0 0 0 0	
4.329E-04	1.430E-01	20	B300	2 1 1 1 2	
4.389E-04	1.450E-01	20	B324	0 0 0 0 0	
4.388E-04	1.450E-01	20	B324	0 0 0 0 0	
4.389E-04	1.450E-01	20	F311	1 2 2 2 1	
4.389E-04	1.450E-01	20	M061	1 0 0 0 2	
4.389E-04	1.450E-01	20	M344	1 0 0 0 2	
4.964E-04	1.640E-01	30	B324	0 0 0 0 0	
4.963E-04	1.640E-01	30	B324	0 0 0 0 0	
4.389E-04	1.450E-01	rt	M161	0 0 0 0 2	

2315. $C_{10}H_{20}$
Cyclodecane
RN: 293-96-9 **MP** (°C)**:** 10
MW: 140.27 **BP** (°C)**:** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-06	3.300E-04	25	T423	0 0 0 0 0	

2316. $C_{10}H_{20}$
n-Pentylcyclopentane
1-Pentylcyclopentane
RN: 3741-00-2 **MP** (°C)**:**
MW: 140.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.198E-07	1.150E-04	25	K119	1 0 0 0 2	
8.198E-07	1.150E-04	25	P051	2 1 1 2 2	
8.198E-07	1.150E-04	25.00	P007	2 1 2 2 2	

2317. $C_{10}H_{20}NO_4PS$
Propetamphos
Methylethyl (E)-3-(((ethylamino)methoxyphosphinothioyl)oxy)-2-butenoate
Safrotin
Seraphos
Zoecon
RN: 31218-83-4 **MP** (°C)**:**
MW: 281.31 **BP** (°C)**:** 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-04	1.100E-01	24	M161	1 0 0 0 2	

2318. $C_{10}H_{20}NO_5PS_2$
Mecarbam
O,O-Diethyl *S*-(*N*-methyl-*N*-carboethoxycarbamoylmethyl) dithiophosphate
RN: 2595-54-2 **MP** (°C)**:**
MW: 329.38 **BP** (°C)**:** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.033E-03	9.990E-01	rt	M061	0 0 0 0 0	
<3.04E-03	<1.00E+00	rt	M161	0 0 0 0 0	

2319. $C_{10}H_{20}N_2S_4$
Disulfiram
Tetraethylthioperoxydicarbonothioic diamide
Tetraethylthiuram disulfide
Antadix
Antabuse
Esperal
RN: 97-77-8 **MP** (°C)**:** 70
MW: 296.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.744E-04	2.000E-01	25	I314	0 0 0 0 0	
1.379E-05	4.090E-03	25	L033	1 0 2 1 2	*sic*
1.012E-03	3.000E-01	ns	N061	0 0 0 0 0	

2320. $C_{10}H_{20}N_6O$
N-(Methoxymethyl)pentamethylmelamine
N-Methylolpentamethylmelamine methyl ether
RN: 64124-15-8 **MP** (°C)**:** 39
MW: 240.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-03	1.500E+00	25	C051	1 2 1 1 1	pH 7, unstable in water

2321. $C_{10}H_{20}O$
Citronellol
3,7-Dimethyl-6-octen-1-ol
Levo-citronellol
β-Citronellol
RN: 106-22-9 **MP** (°C)**:**
MW: 156.27 **BP** (°C)**:** 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-03	2.000E-01	25	M350	1 0 1 1 1	

2322. $C_{10}H_{20}O$
Decanal
Cuprylaldehyde
RN: 112-31-2 **MP** (°C)**:** 7
MW: 156.27 **BP** (°C)**:** 207–209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.983E-05	1.560E-02	25	L450	0 0 0 0 0	

2323. $C_{10}H_{20}O$
Menthol
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-
3-*p*-Menthanol
RN: 89-78-1 **MP** (°C)**:** 42
MW: 156.27 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-03	4.000E-01	20	F300	1 0 0 0 2	
2.920E-03	4.563E-01	25	I019	1 0 1 2 2	
8.600E-03	1.344E+00	37	E028	1 0 1 1 1	

2324. $C_{10}H_{20}O$
l-Menthol
1-Isopropyl-4-methyl cyclohexan-2-ol
1-Methyl-4-isopropyl cyclohexan-3-ol
(1R,2S,5R)-(–)-Menthol
5-Methyl-2-isopropyl hexahydrophenol
Cyclohexanol
RN: 2216-51-5 **MP** (°C)**:** 44
MW: 156.27 **BP** (°C)**:** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	6.251E-01	25	A401	1 0 2 2 0	

2325. $C_{10}H_{20}O_2$
3-Hydroxy-2-ethyl-5-propyl-5-methyltetrahydrofuran
3-Furanol, 2-ethyltetrahydro-5-methyl-5-propyl-
RN: 29839-73-4 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2326. $C_{10}H_{20}O_2$
3-Hydroxy-2,2-dimethyl-5,5-diethyltetrahydrofuran
3-Furanol, 5,5-diethyltetrahydro-2,2-dimethyl-
RN: 29839-77-8 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2327. $C_{10}H_{20}O_2$
3-Hydroxy-2,5,5-triethyltetrahydrofuran
3-Furanol, 2,5,5-triethyltetrahydro-
RN: 29839-70-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2328. $C_{10}H_{20}O_2$
3-Hydroxy-2,5-dipropyltetrahydrofuran
3-Furanol, 2,5-dipropyltetrahydro-
RN: 30003-27-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2329. $C_{10}H_{20}O_2$
3-Hydroxy-2-butyl-5,5-methyltetrahydrofuran
3-Furanol, 2-butyltetrahydro-5,5-dimethyl-
RN: 29839-71-2 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2330. $C_{10}H_{20}O_2$
3-Hydroxy-2-pentyl-5-methyltetrahydrofuran
3-Furanol, 5-methyltetrahydro-2-pentyl-
RN: 29848-45-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2331. $C_{10}H_{20}O_2$
3-Hydroxy-2-propyl-5-methyl-5-ethyltetrahydrofuran
3-Furanol, 5-ethyltetrahydro-5-methyl-2-propyl-
RN: 29839-72-3 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2332. $C_{10}H_{20}O_2$
n-Capric acid
Caprinsaeure
Decanoic acid
Nonanecarboxylic acid
RN: 334-48-5 **MP** (°C)**:** 31.4
MW: 172.27 **BP** (°C)**:** 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.515E-04	9.500E-02	0	B136	1 0 2 1 1	
1.509E-04	2.600E-02	15	F300	1 0 0 0 1	
2.902E-04	5.000E-02	20	A011	1 2 1 1 1	
9.462E-04	1.630E-01	20	B136	1 0 2 1 2	
8.706E-04	1.500E-01	20	D041	1 0 0 0 1	
8.706E-04	1.500E-01	20.0	R001	1 1 1 1 1	
3.590E-04	6.184E-02	25	J001	1 0 2 1 2	
1.115E-03	1.920E-01	30	B136	1 0 2 1 2	
3.715E-04	6.400E-02	30	E005	2 1 1 2 1	
1.045E-03	1.800E-01	30.0	R001	1 1 1 1 1	
1.294E-03	2.230E-01	40	B136	1 0 2 1 2	
4.179E-04	7.200E-02	40	E005	2 1 1 2 1	
1.335E-03	2.300E-01	45	B136	1 0 2 1 1	
1.335E-03	2.299E-01	45.0	R001	1 1 1 1 1	
4.702E-04	8.100E-02	50	E005	2 1 1 2 1	
5.000E-04	8.613E-02	50	J001	1 0 2 1 2	
1.567E-03	2.700E-01	60	B136	1 0 2 1 1	
5.805E-04	1.000E-01	60	E005	2 1 1 2 2	
1.567E-03	2.699E-01	60.0	R001	1 1 1 1 1	
5.514E-04	9.499E-02	.0	R001	1 1 1 1 1	

2333. $C_{10}H_{20}O_2$
3-Hydroxy-5,5-dipropyltetrahydrofuran
3-Furanol, 5,5-dipropyltetrahydro-
RN: 29839-54-1 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2334. $C_{10}H_{20}O_2$
3-Hydroxy-5,5-diisopropyltetrahydrofuran
3-Furanol, 5,5-diisopropyltetrahydro-
RN: 29839-55-2 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2335. $C_{10}H_{20}O_2$
3-Hydroxy-2,5-dimethyl-2,5-diethyltetrahydrofuran
3-Furanol, 2,5-diethyltetrahydro-2,5-dimethyl-
RN: 30010-09-4 **MP** (°C)**:**
MW: 172.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-01	1.961E+01	rt	B066	0 2 0 0 0	

2336. $C_{10}H_{20}O_2.H_2O$
Terpin (monohydrate)
Terpin-hydrat
RN: 2451-01-6 **MP** (°C)**:** 116
MW: 190.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.102E-02	4.000E+00	15	F300	1 0 0 0 0	
1.799E-02	3.424E+00	25	M012	1 0 2 1 2	
1.661E-01	3.160E+01	100	F300	1 0 0 0 2	

2337. $C_{10}H_{20}O_3$
1,3-Dioxolane-4-methanol, 2-methyl-2-pentyl
2-Heptanone, cyclic (hydroxymethyl)ethylene acetal
2-Methyl-2-*n*-amyl-4-hydroxymethyl-1,3-dioxolane
2-Methyl-2-pentyl-1,3-dioxolane-4-methanol
RN: 4361-59-5 **MP** (°C)**:**
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.090E-02	9.583E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2338. $C_{10}H_{20}O_3$
n-Amyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, pentyl ester
RN: 14144-36-6 **MP** (°C)**:**
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.366E-03	1.199E+00	25	D002	1 2 1 1 1	

2339. $C_{10}H_{20}O_4$
Butyl carbitol acetate
Diethylene glycol acetate butyl ether
Diethylene glycol butyl ether acetate
Diglykol-monobutylaether-acetat
RN: 124-17-4 **MP** (°C)**:** –32
MW: 204.27 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.709E-02	1.575E+01	20	D052	1 1 0 0 1	
1.792E-01	3.661E+01	20	M062	1 0 0 0 1	

2340. $C_{10}H_{21}NOS$
Pebulate
S-Propyl butylethylthiocarbamate
RN: 1114-71-2 **MP** (°C)**:** <25
MW: 203.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-04	6.000E-02	20	M161	1 0 0 0 1	
4.524E-04	9.200E-02	21	F019	1 0 0 0 1	
4.524E-04	9.200E-02	21	M061	1 0 0 0 1	
2.951E-04	6.000E-02	ns	B200	0 0 0 0 1	
2.951E-04	6.001E-02	ns	S460	0 0 0 0 0	

2341. $C_{10}H_{21}NOS$
Vernolate
S-Propyl dipropylthiocarbamate
Carbamic acid, dipropylthio-, *S*-propyl ester
Carbamate, *n*-propyl-di-*n*-propylthio-
Vernam
RN: 1929-77-7 **MP** (°C)**:** <25
MW: 203.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.426E-04	9.000E-02	20	B200	1 0 0 0 1	
5.262E-04	1.070E-01	21	F019	1 0 0 0 2	
5.262E-04	1.070E-01	21	M161	1 0 0 0 2	
<4.92E-04	<1.00E-01	ns	B185	0 0 0 0 0	
4.917E-04	9.999E-02	ns	M061	0 0 0 0 0	

2342. $C_{10}H_{22}$
2,2-Dimethyloctane
RN: 15869-87-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-07	1.067E-04	ns	S460	0 0 0 0 0	

2343. $C_{10}H_{22}$
n-Decane
Decane
Decyl hydride
RN: 124-18-5 **MP** (°C)**:** –30.0
MW: 142.29 **BP** (°C)**:** 174.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-07	1.976E-05	20	B165	1 0 1 1 1	
1.124E-07	1.600E-05	25	B069	1 0 1 1 1	
1.389E-07	1.976E-05	25	F004	0 0 0 0 0	
3.655E-07	5.200E-05	25	M003	1 0 2 2 1	
3.655E-07	5.200E-05	25	M040	1 0 0 1 1	
3.233E-07	4.600E-05	25	T423	0 0 0 0 0	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 2	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 0	
3.655E-07	5.200E-05	ns	H123	0 0 0 0 0	

2344. $C_{10}H_{22}$
4,4-Dimethyloctane
RN: 15869-95-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 157.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E-05	2.200E-03	20	M337	2 1 2 2 1	
7.278E-07	1.036E-04	ns	S460	0 0 0 0 0	

2345. $C_{10}H_{22}$
2,3-Dimethyloctane
RN: 7146-60-3 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.117E-07	7.281E-05	ns	S460	0 0 0 0 0	

2346. $C_{10}H_{22}$
2,6-Dimethyloctane
RN: 2051-30-1 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.266E-07	8.916E-05	ns	S460	0 0 0 0 0	

2347. $C_{10}H_{22}$
3,6-Dimethyloctane
RN: 15869-94-0 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.109E-07	8.693E-05	ns	S460	0 0 0 0 0	

2348. $C_{10}H_{22}$
3-Ethyloctane
RN: 5881-17-4 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-07	6.519E-05	ns	S460	0 0 0 0 0	

2349. $C_{10}H_{22}$
4-Methylnonane
4-Methylnonane(DL)
RN: 17301-94-9 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.764E-07	6.779E-05	ns	S460	0 0 0 0 0	

2350. $C_{10}H_{22}$
3,3-Dimethyloctane
RN: 4110-44-5 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.998E-07	8.534E-05	ns	S460	0 0 0 0 0	

2351. $C_{10}H_{22}$
4-Ethyloctane
RN: 15869-86-0 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.297E-07	7.536E-05	ns	S460	0 0 0 0 0	

2352. $C_{10}H_{22}$
3,5-Dimethyloctane
RN: 15869-93-9 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.546E-07	9.315E-05	ns	S460	0 0 0 0 0	

2353. $C_{10}H_{22}$
3-Methylnonane
3-Methylnonane(DL)
RN: 5911-04-6 **MP** (°C)**:**
MW: 142.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.295E-07	6.112E-05	ns	S460	0 0 0 0 0	

2354. $C_{10}H_{22}O$
Decanol
RN: 36729-58-5 **MP** (°C)**:**
MW: 158.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.166E-02	24	H345	0 0 0 0 0	

2355. $C_{10}H_{22}O$
n-Decyl alcohol
Alcohol C-10
Nonyl acarbinol
Capric alcohol
RN: 36729-58-5 **MP** (°C)**:**
MW: 158.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	4.258E-02	20	H330	0 0 0 0 0	
2.000E-04	3.166E-02	24	H345	2 0 2 2 2	
2.340E-04	3.704E-02	25	K025	2 2 1 1 2	
2.527E-05	4.000E-03	40	W305	1 0 0 1 0	EFG
3.000E-04	4.748E-02	ns	H012	0 2 2 0 0	

2356. $C_{10}H_{23}O_2PS_2$
Cadusafos
Ebufos
Taredan
Rugby
Apache
O-ethyl *S,S*-bis(1-methylpropyl) phosphorodithioate
RN: 95465-99-9 **MP** (°C)**:**
MW: 270.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.162E-04	2.477E-01	ns	S460	0 0 0 0 0	

2357. $C_{10}H_{23}O_3P$
Ethyl dibutyl phosphonate
Dibutyl ethyl phosphonate
RN: 2404-58-2 **MP** (°C)**:**
MW: 222.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.699E-02	6.000E+00	25	B070	1 2 0 1 0	
5.849E-02	1.300E+01	25	B070	1 2 0 1 1	

2358. $C_{10}H_{23}O_4P$
Dibutyl ethyl phosphate
RN: 7242-58-2 **MP** (°C)**:**
MW: 238.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-02	3.400E+00	25	B070	1 2 2 1 1	

2359. $C_{10}Cl_{10}O$

Chlordecone
Kepone
1,2,3,5,6,7,8,9,10,10-Decachloropentacyclo[5.2.1.0(2,6).0(3,9).0(5,8)]decano-4-one
Merex
Decachloroketone
RN: 143-50-0 **MP** (°C)**:**
MW: 490.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.153E-03	4.000E+00	100	M161	1 0 0 0 0	
6.166E-06	3.025E-03	ns	R424	0 0 0 0 0	
6.166E-06	3.025E-03	ns	R427	0 0 0 0 0	

2360. $C_{10}Cl_{12}$

Mirex
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene dimer
Bichlorendo
Ferriamicide
Dechlorane 4070
RN: 2385-85-5 **MP** (°C)**:**
MW: 545.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-07	8.450E-05	24.99	K436	0 0 0 0 0	
1.397E-10	7.619E-08	25	H434	0 0 0 0 0	
1.558E-07	8.500E-05	25	M134	1 2 1 1 1	
1.741E-07	9.500E-05	ns	M110	0 0 0 0 0	EFG
1.660E-07	9.054E-05	ns	R427	0 0 0 0 0	

2361. $C_{11}H_6BrNS$

1-Bromo-2-naphthylisothiocyanate
RN: 2392-80-5 **MP** (°C)**:**
MW: 264.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-05	1.268E-02	25	D019	1 1 1 1 1	

2362. $C_{11}H_6O_3$

Psoralen
7H-Furo[3,2-g][1]benzopyran-7-one
RN: 66-97-7 **MP** (°C)**:** 158–161
MW: 186.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-04	6.516E-02	25	A355	0 0 0 0 0	

2363. $C_{11}H_7Cl_2NO_3$
Pyoluteorin
RN: **MP** (°C)**:**
MW: 272.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.442E-01	5.0	L451	0 0 0 0 0	
5.600E-04	1.524E-01	10	L451	0 0 0 0 0	
6.300E-04	1.714E-01	15.0	L451	0 0 0 0 0	
7.500E-04	2.041E-01	20.0	L451	0 0 0 0 0	
7.900E-04	2.150E-01	25.0	L451	0 0 0 0 0	
9.600E-04	2.612E-01	30.0	L451	0 0 0 0 0	
9.900E-04	2.694E-01	35.0	L451	0 0 0 0 0	
1.150E-03	3.129E-01	40.0	L451	0 0 0 0 0	
1.290E-03	3.510E-01	45.0	L451	0 0 0 0 0	
1.500E-03	4.081E-01	50.0	L451	0 0 0 0 0	
1.590E-03	4.326E-01	55.0	L451	0 0 0 0 0	
1.730E-03	4.707E-01	60.0	L451	0 0 0 0 0	

2364. $C_{11}H_7FN_2O_3$
3-Benzoyl-5-fluorouracil
RN: 61251-77-2 **MP** (°C)**:** 169–170
MW: 234.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.551E-03	1.300E+00	22	B321	0 0 0 0 0	pH 4.0
5.551E-03	1.300E+00	22	B332	1 1 0 0 1	pH 4.0

2365. $C_{11}H_7FN_2O_4$
3-Phenyloxycarbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
3-Phenyloxycarbonyl-5-fluorouracil
RN: 66999-97-1 **MP** (°C)**:** 169–170
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.995E-04	1.500E-01	22	B321	0 0 0 0 0	pH 4.0

2366. $C_{11}H_7FN_2O_4$
1-Phenyloxycarbonyl-5-fluorouracil
RN: 75410-28-5 **MP** (°C)**:**
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-03	9.000E-01	22	B332	1 1 0 0 1	pH 4.0

2367. $C_{11}H_7NS$
2-Naphthyl isothiocyanate
2-Isothiocyanatonaphthalene
β-Naphthyl mustard oil
RN: 1636-33-5 **MP** (°C)**:**
MW: 185.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	6.669E-03	25	D019	1 1 1 1 1	

2368. $C_{11}H_7NS$
1-Naphthyl isothiocyanate
1-Isothiocyanatonaphthalene
α-Naphthyl mustard oil
Kesscocide
ANI
ANIT
RN: 551-06-4 **MP** (°C)**:** 58.0
MW: 185.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	4.631E-03	25	D019	1 1 1 1 1	

2369. $C_{11}H_8N_2$
β-Carboline
β-Carbolin
Norharmane
9H-Pyrido(3,4-b)indole
RN: 244-63-3 **MP** (°C)**:** 199
MW: 168.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E+01	2.340E+03	16	B413	1 0 2 2 1	
1.601E+01	2.693E+03	17	B413	1 0 2 2 1	
2.535E+01	4.264E+03	37	B413	1 0 2 2 1	
2.561E+01	4.308E+03	38	B413	1 0 2 2 1	
2.916E+01	4.905E+03	45	B413	1 0 2 2 1	

2370. $C_{11}H_8N_4O_4$
Orotic acid nicotinmide
RN: **MP** (°C)**:** 252–253
MW: 260.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-02	1.769E+01	25	N018	0 0 0 0 0	

2371. $C_{11}H_8O_2$
2-Naphthoic acid
β-Naphthoic acid
2-Naphthalenecarboxylic acid
RN: 93-09-4 **MP** (°C)**:**
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.238E-02	25	M149	2 2 2 2 1	intrinsic, *sic*
1.617E-06	2.785E-04	30	K148	1 1 0 0 2	
2.323E-06	4.000E-04	40	K148	1 1 0 0 1	
3.165E-06	5.450E-04	50	K148	1 1 0 0 2	
3.949E-06	6.800E-04	60	K148	1 1 0 0 2	
4.652E-06	8.010E-04	70	K148	1 1 0 0 2	
5.459E-06	9.400E-04	80	K148	1 1 0 0 2	
6.261E-06	1.078E-03	90	K148	1 1 0 0 2	

2372. $C_{11}H_8O_2$
Menadione
2-Methyl-1,4-naphthoquinone
Vitamin K3
Kativ-G
Panosine
Menaphthone
RN: 58-27-5 **MP** (°C)**:** 106
MW: 172.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.291E-04	1.600E-01	25	P096	0 0 0 0 0	
6.969E-04	1.200E-01	30	K090	1 2 2 2 0	EFG
8.700E-04	1.498E-01	30	O321	0 0 0 0 0	
8.710E-04	1.500E-01	30	O321	0 0 0 0 0	
9.291E-04	1.600E-01	30.00	E033	1 0 2 1 0	EFG
8.888E-04	1.530E-01	33	D404	2 1 2 2 2	
8.768E-04	1.510E-01	33	D404	2 1 2 2 2	
1.161E-03	2.000E-01	37.00	E033	1 0 2 1 0	EFG

2373. $C_{11}H_8O_3$
8-Hydroxypsoralon
RN: **MP** (°C)**:**
MW: 188.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	1.148E-01	25	A355	0 0 0 0 0	

2374. $C_{11}H_8O_3$
2-Methoxy-1,4-naphthoquinone
1,4-Naphthalenedione, 2-methoxy-
2-Methoxy-1,4-naphthoquinone
RN: 2348-82-5 **MP** (°C)**:**
MW: 188.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-04	3.123E-02	ns	R427	0 0 0 0 0	

2375. $C_{11}H_9ClO_2S$
Tianafac
RN: 51527-19-6 **MP** (°C)**:**
MW: 240.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.444E-04	3.476E-02	25	C314	0 0 0 0 0	
1.442E-04	3.470E-02	25	C314	0 0 0 0 0	

2376. $C_{11}H_9Cl_2NO_2$
Barban
4-Chloro-2-butynyl-*N*-(3-chlorophenyl)carbamate
4-Chloro-2-butynyl-*m*-chlorocarbanilate
RN: 101-27-9 **MP** (°C)**:** 75
MW: 258.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.262E-05	1.100E-02	25	B200	1 0 0 0 2	
4.262E-05	1.100E-02	25	M161	1 0 0 0 1	
3.874E-05	1.000E-02	ns	H042	0 0 0 0 1	
4.262E-04	1.100E-01	ns	M061	0 0 0 0 2	

2377. $C_{11}H_9Cl_4NO_4$
OCS-21693
TMMT
Methyl-2,3,5,6-tetrachloro-*N*-methoxy-*N*-methylterephthalamate
RN: 14419-01-3 **MP** (°C)**:** 96
MW: 361.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	5.000E-03	25	B200	1 0 0 0 0	

2378. $C_{11}H_9I_3N_2O_4$
3,5-Diacetylamino-2,4,6-triiodobenzoic acid
Iothalamic acid
Diatrazoic acid
RN: 117-96-4 **MP** (°C)**:**
MW: 613.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.144E-01	5.000E+02	25	L100	1 0 0 0 2	
9.773E-01	6.000E+02	50	L100	1 0 0 0 2	
1.189E+00	7.297E+02	90	L100	1 0 0 0 2	
2.557E-03	1.570E+00	ns	H055	0 0 0 0 0	

2379. $C_{11}H_{10}$
2-Methylnaphthalene
2-Methyl naphthalene
β-Methyl naphthalenes
RN: 91-57-6 **MP** (°C)**:** 35
MW: 142.20 **BP** (°C)**:** 241.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	2.460E-02	25	E004	2 1 2 2 2	
1.828E-04	2.600E-02	25	L332	1 1 1 1 0	
1.786E-04	2.540E-02	25	M064	1 1 2 2 2	
1.800E-04	2.560E-02	25	M342	1 0 1 1 1	
1.758E-04	2.500E-02	25	O320	0 0 0 0 0	
1.786E-04	2.540E-02	ns	H123	0 0 0 0 0	
8.000E-05	1.138E-02	ns	L060	0 0 0 0 0	
1.786E-04	2.540E-02	ns	M344	0 0 0 0 2	

2380. $C_{11}H_{10}$
1-Methylnaphthalene
1-Methyl naphthalene
1-Methyl-napthalene
α-Methyl naphthalenes
α-Methylnaphthalene
RN: 90-12-0 **MP** (°C)**:** –22
MW: 142.20 **BP** (°C)**:** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E-04	2.473E-02	4	D351	1 2 1 1 2	
1.600E-04	2.275E-02	10	S076	2 2 2 2 1	
2.000E-04	2.844E-02	14	S076	2 2 2 2 1	
1.195E-04	1.700E-02	20	A050	1 0 1 1 1	
2.145E-04	3.050E-02	20	B318	0 0 0 0 0	EFG
2.124E-04	3.020E-02	20	B356	0 0 0 0 0	
2.000E-04	2.844E-02	20	S076	2 2 2 2 1	
2.100E-04	2.986E-02	21	A057	2 1 2 2 1	

(*continued*)

2380. $C_{11}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-04	3.539E-02	25	D351	1 2 1 1 2	
1.814E-04	2.580E-02	25	E004	2 1 2 2 2	
1.899E-04	2.700E-02	25	L332	1 1 1 1 0	
2.004E-04	2.850E-02	25	M064	1 1 2 2 2	
2.000E-04	2.844E-02	25	M342	1 0 1 1 2	
2.100E-04	2.986E-02	25	S076	2 2 2 2 1	
2.440E-04	3.470E-02	28	B348	2 2 2 2 2	
2.955E-04	4.203E-02	40	D351	1 2 1 1 2	
2.004E-04	2.850E-02	ns	H123	0 0 0 0 0	
1.600E-04	2.275E-02	ns	L060	0 0 0 0 1	
2.004E-04	2.850E-02	ns	M344	0 0 0 0 2	

2381. $C_{11}H_{10}BrN_3O_2S$
5-Sulfanilamido-2-bromopyridine
Benzenesulfonamide, 4-amino-*N*-(2-bromo-5-pyridinyl)-
RN: 17103-43-4 **MP** (°C)**:**
MW: 328.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-04	1.220E-01	37	R058	1 2 1 1 2	

2382. $C_{11}H_{10}BrN_3O_2S$
2-Sulfanilamido-5-bromopyridine
Benzenesulfonamide, 4-amino-*N*-(5-bromo-2-pyridinyl)-
RN: 16805-99-5 **MP** (°C)**:**
MW: 328.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-04	3.800E-02	37	R058	1 2 1 1 1	

2383. $C_{11}H_{10}ClNO_2$
Chlorbupham
1-Methylpropyn-2-yl *N*-(*m*-chlorophenyl)carbamate
Chlorbufam
Bi-PC
RN: 1967-16-4 **MP** (°C)**:** 45.5
MW: 223.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.414E-03	5.400E-01	20	B185	0 0 0 0 0	
2.414E-03	5.400E-01	20	M161	1 0 0 0 2	

2384. $C_{11}H_{10}ClN_3O_2S$
5-Sulfanilamido-2-chloropyridine
*N*1-(6-Chloro-3-pyridyl)sulfanilamide
RN: 34392-82-0 **MP** (°C)**:**
MW: 283.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.344E-04	1.800E-01	37	R058	1 2 1 1 1	

2385. $C_{11}H_{10}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid allyl ester
Allyl 2,4-dichlorophenoxyacetate
RN: 58965-05-2 **MP** (°C)**:**
MW: 261.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	3.722E-02	ns	M120	0 0 1 1 2	

2386. $C_{11}H_{10}IN_3O_2S$
2-Sulfanilamido-5-iodopyridine
Benzenesulfonamide, 4-amino-*N*-(5-iodo-2-pyridinyl)-
RN: 71119-21-6 **MP** (°C)**:**
MW: 375.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-05	1.300E-02	37	R058	1 2 1 1 1	

2387. $C_{11}H_{10}N_2O$
3-*o*-Toluoxypyridazine
Credazine
3-(2-Methylphenoxy)-pyridazine
RN: 14491-59-9 **MP** (°C)**:** 78
MW: 186.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	1.996E+00	ns	B100	0 0 0 0 0	
1.074E-02	2.000E+00	rt	M161	0 0 0 0 0	

2388. $C_{11}H_{10}N_2O$
Vasicinone
Pyrrolo[2,1-b]quinazolin-9(1H)-one, 2,3-dihydro-3-hydroxy-, (3*S*)-
(–)-Vasicinone
L-Vasicinone
RN: 486-64-6 **MP** (°C)**:** 204
MW: 186.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-03	1.597E+00	25	B194	2 2 2 2 1	

2389. $C_{11}H_{10}N_2O_3$
Phenylmethylbarbituric acid
Barbituric acid, 5-methyl-5-phenyl
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-phenyl
2,4,6-Trioxo-5-methyl-5-phenylhexahydropyrimidine
Heptobarbital
RN: 76-94-8 **MP** (°C)**:** 226
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-03	7.594E-01	20	J030	1 2 2 2 1	
4.170E-03	9.100E-01	25	P350	0 0 0 0 0	intrinsic
6.133E-03	1.338E+00	37	J030	1 2 2 2 2	

2390. $C_{11}H_{10}N_2S$
1-Naphthylthiourea
ANTU
RN: 86-88-4 **MP** (°C)**:** 198
MW: 202.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.966E-03	6.000E-01	rt	M161	0 0 0 0 2	

2391. $C_{11}H_{10}N_4O_4S$
2-Sulfanilamido-5-nitropyridine
Benzenesulfonamide, 4-amino-*N*-(5-nitro-2-pyridinyl)-
RN: 39588-36-8 **MP** (°C)**:**
MW: 294.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-04	3.700E-02	37	R058	1 2 1 1 1	

2392. $C_{11}H_{11}ClO_3$
Alclofenac
(4-Allyloxy-3-chlorophenyl)acetic acid
(3-Chloro-4-allyloxyphenyl)acetic acid
RN: 22131-79-9 **MP** (°C)**:**
MW: 226.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.850E-05	1.099E-02	5	F306	1 0 1 2 2	intrinsic
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
6.200E-05	1.405E-02	25	F306	1 0 1 2 2	intrinsic
8.000E-05	1.813E-02	37	F306	1 0 1 2 2	intrinsic

2393. $C_{11}H_{11}N$
2,4-Dimethylquinoline
Quinoline, 2,4-dimethyl-
RN: 1198-37-4 **MP** (°C)**:** 264
MW: 157.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	K119	1 0 0 0 2	

2394. $C_{11}H_{11}N$
2,7-Dimethylquinoline
Quinoline, 2,7-dimethyl-
RN: 93-37-8 **MP** (°C)**:** 58
MW: 157.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	P051	2 1 1 2 2	
1.142E-02	1.795E+00	25.00	P007	2 1 2 2 2	

2395. $C_{11}H_{11}NO$
Aziridine, 1-(1-oxo-3-phenyl-2-propenyl)-
N-Cyclopropylcinnamamide
RN: 53162-40-6 **MP** (°C)**:**
MW: 173.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.150E-03	5.456E-01	ns	H350	0 0 0 0 0	

2396. $C_{11}H_{11}NO_2$

Phensuximide
Milontin
N-Methyl-2-phenyl-succinimide
RN: 86-34-0 **MP** (°C)**:** 71–73
MW: 189.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-02	4.200E+00	25	P061	0 0 0 0 0	

2397. $C_{11}H_{11}NO_2S$

Butyric acid, *p*-isothiocyanatophenyl ester
RN: 96933-13-0 **MP** (°C)**:**
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.814E-02	25	K032	2 2 0 1 1	

2398. $C_{11}H_{11}NO_4$

Acetamide, *N*-acetyl-2-(benzoyloxy)-
RN: 68659-48-3 **MP** (°C)**:** 104.5
MW: 221.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.978E-03	8.800E-01	22	N317	1 1 2 1 2	

2399. $C_{11}H_{11}NO_4S$

4-Thiazolidinecarboxylic acid, 2-(4-carboxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(4-carboxyphenyl)-
RN: 118845-10-6 **MP** (°C)**:**
MW: 253.28 **BP** (°C)**:** 551.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.520E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2400. $C_{11}H_{11}NO_5$
Benzoxydiglycine
RN: **MP** (°C)**:**
MW: 237.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E-02	3.300E+00	25.1	N026	0 0 0 0 0	

2401. $C_{11}H_{11}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-amino-2-oxoethyl ester
(*O*-Acetylsalicyloyloxy)acetamide
RN: 50785-22-3 **MP** (°C)**:** 128.5
MW: 237.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-02	3.840E+00	21	N335	0 0 0 0 0	

2402. $C_{11}H_{11}N_3OS$
Seedvax
2-Amino-4-methyl-5-carboxanilidothiazole
RN: 21452-14-2 **MP** (°C)**:** 221
MW: 233.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.282E-03	9.990E-01	ns	M061	0 0 0 0 0	

2403. $C_{11}H_{11}N_3O_2S$
Sulfapyridine
2-(Aminobenzene-4′-sulfamido)-pyridine
2-[Aminobenzol-4′-sulfamid]-pyridin
Sulphapyridine
2-Sulfapyridine
N-(2-Pyridyl)sulfanilamide
RN: 144-83-2 **MP** (°C)**:** 192
MW: 249.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-04	1.700E-01	16	H114	1 0 0 0 2	
2.006E-03	5.000E-01	20	C103	1 2 0 0 2	
1.323E-03	3.299E-01	20	D041	1 0 0 0 1	
8.023E-04	2.000E-01	20	F073	1 2 2 2 2	
1.075E-03	2.680E-01	25	C102	2 0 2 2 2	
1.049E-03	2.615E-01	25	M440	0 0 0 0 0	
1.645E-03	4.100E-01	35	H114	1 0 0 0 1	

(*continued*)

2403. $C_{11}H_{11}N_3O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-03	4.860E-01	37	C102	2 0 2 2 2	
1.805E-03	4.500E-01	37	D084	1 0 1 0 1	
1.985E-03	4.948E-01	37	F072	1 0 0 0 2	
1.985E-03	4.948E-01	37	F075	1 0 2 2 2	
2.006E-03	5.000E-01	37	F300	1 0 0 0 0	
4.047E-03	1.009E+00	37	G037	2 2 2 1 0	EFG, form V
6.128E-03	1.528E+00	37	G073	2 2 2 1 0	EFG, amorphous
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form II
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form I
2.090E-03	5.210E-01	37	K095	2 0 0 0 2	intrinsic
2.447E-03	6.100E-01	37	M057	1 0 0 0 2	pH 5.5
2.607E-03	6.500E-01	37	R044	0 0 0 0 0	
6.417E-04	1.600E-01	37.50	M142	1 0 0 0 1	
2.165E-03	5.397E-01	37.50	M142	1 0 0 0 1	
2.006E-03	5.000E-01	38	K006	1 0 0 0 2	
4.412E-03	1.100E+00	40	C103	1 2 0 0 2	
4.212E-02	1.050E+01	100	C103	1 2 0 0 2	
3.972E-02	9.901E+00	100	D041	1 0 0 0 0	
1.995E-03	4.974E-01	ns	R427	0 0 0 0 0	
1.484E-03	3.699E-01	rt	N015	0 0 2 2 2	

2404. $C_{11}H_{11}N_3O_3S_2$

Acetyl sulfathiazole
Sulfathiazol acetyle
*N*4-Acetylsulfathiazole
*N*4-Acetylsulphathiazole

RN: 127-76-4 **MP** (°C)**:**
MW: 297.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.363E-04	1.000E-01	37	D084	1 0 1 0 1	
2.186E-04	6.500E-02	37	F075	1 0 2 2 1	
2.354E-04	7.000E-02	37	L091	1 0 0 0 0	pH 5.5
1.951E-04	5.800E-02	37	M057	1 0 0 0 1	pH 5.5
2.018E-04	6.000E-02	37.50	M142	1 0 0 0 0	
2.388E-04	7.100E-02	38	K006	1 0 0 0 1	

2405. $C_{11}H_{11}N_3O_3S$

5-Sulfanilamido-2-hydroxypyridine

RN: 71119-20-5 **MP** (°C)**:**
MW: 265.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.725E-03	2.580E+00	37	R058	1 2 1 1 1	

2406. $C_{11}H_{11}N_5$
Phenazopyridine
3-(Phenylazo)-2,6-pyridinediamine
RN: 94-78-0 **MP** (°C)**:** 235
MW: 213.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.240E+00	9.042E+02	25	B443	0 0 0 0 0	
1.738E-04	3.706E-02	ns	R427	0 0 0 0 0	

2407. $C_{11}H_{12}ClNO_4$
Chloroethyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl 2-chloroethyl ester
Acetanilide, 4′-hydroxy-, 2-chloroethyl carbonate (ester)
RN: 17243-29-7 **MP** (°C)**:** 122.5–123
MW: 257.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.514E-03	3.900E-01	37	D029	0 0 0 0 0	

2408. $C_{11}H_{12}Cl_2N_2O_5$
Chloramphenicol
D-(–)-Threo-1-(*p*-nitrophenyl)-2-dichloroacetamido-1,3-propanediol
Amphicol
Leukomycin
Cloramical
Intramyctin
RN: 56-75-7 **MP** (°C)**:** 150.5
MW: 323.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.717E-03	2.494E+00	20	D041	1 0 0 0 1	
5.570E-03	1.800E+00	23	M168	2 0 0 0 0	EFG
1.200E-02	3.878E+00	25	A352	0 0 0 0 0	
7.717E-03	2.494E+00	25	I312	0 0 0 0 0	
1.156E-02	3.736E+00	25.5	J011	1 0 2 1 2	pH 4.7
1.370E-02	4.427E+00	30	K020	1 0 1 1 0	EFG
1.238E-02	4.000E+00	37	G010	1 0 1 1 0	EFG
7.737E-03	2.500E+00	ns	K444	0 0 0 0 0	

2409. $C_{11}H_{12}Cl_2O_3$
2,4-D Isopropyl ester
2,4-D-Isopropyl ester
2,4-Dichlorophenoxyacetic acid isopropyl ester
2,4-Dichlorophenoxyacetic acid *iso*-propyl ester
RN: 94-11-1 **MP** (°C)**:**
MW: 263.12 **BP** (°C)**:** 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.736E-02	ns	M120	0 0 1 1 2	
1.419E-04	3.734E-02	ns	M120	0 0 1 1 2	

2410. $C_{11}H_{12}I_3NO_2$
Iopanoic acid
β-(3-Amino-2,4,6-triiodophenyl)-α-ethylpropionic acid
Bilijodon
Cholevid
Choladine
Colepax
RN: 96-83-3 **MP** (°C)**:** 155.2
MW: 570.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	3.483E-01	37	J016	1 0 0 0 1	pH 7.4
2.627E-05	1.500E-02	ns	H055	0 0 0 0 0	

2411. $C_{11}H_{12}NO_4PS_2$
Phosmet
Phosphorodithioic scid *S*-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] *O,O*-dimethyl ester
Decemthion
Smidan
Appa
Imidan
RN: 732-11-6 **MP** (°C)**:**
MW: 317.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-05	2.440E-02	20	B300	2 1 1 1 2	
7.878E-05	2.500E-02	25	M061	1 0 0 0 1	
7.878E-05	2.500E-02	25	M161	1 0 0 0 1	
7.878E-05	2.500E-02	ns	F071	0 1 2 1 1	
7.943E-05	2.521E-02	ns	R427	0 0 0 0 0	

2412. $C_{11}H_{12}N_2O$

Antipyrine
Antipyrin
2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one
1,2-Dihydro-1,5-dimethyl-2-phenyl-3H-pyrazol-3-one
Phenazone

RN: 60-80-0 **MP** (°C)**:** 114
MW: 188.23 **BP** (°C)**:** 319

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E+00	2.918E+02	2.5	K075	1 0 0 0 2	
1.968E+00	3.705E+02	4.62	M109	2 1 1 1 0	EFG
1.472E-01	2.771E+01	5	L089	1 0 0 0 2	*sic*
1.613E+00	3.036E+02	6.1	K075	1 0 0 0 2	
1.777E-01	3.344E+01	10	L089	1 0 0 0 2	*sic*
2.084E+00	3.922E+02	11.74	M109	2 1 1 1 0	EFG
2.261E+00	4.256E+02	14.20	M109	2 1 1 1 0	EFG
1.771E+00	3.333E+02	20	D041	1 0 0 0 0	
2.205E-01	4.150E+01	20	L089	1 0 0 0 2	*sic*
2.472E+00	4.654E+02	20.96	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	25	L089	1 0 0 0 2	*sic*
3.294E+00	6.200E+02	25	P012	0 0 0 0 0	
3.294E+00	6.200E+02	25	P016	1 0 0 1 2	
3.559E+00	6.700E+02	25	P020	2 0 1 1 2	
2.717E+00	5.114E+02	25.35	M109	2 1 1 1 0	EFG
3.020E+00	5.685E+02	29.87	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	30	L089	1 0 0 0 2	*sic*
2.983E-01	5.616E+01	35	L089	1 0 0 0 2	*sic*
3.968E+00	7.468E+02	39.34	M109	2 1 1 1 0	EFG
3.359E-01	6.323E+01	40	L089	1 0 0 0 2	*sic*
5.637E-01	1.061E+02	50	L089	1 0 0 0 2	*sic*
1.493E+00	2.811E+02	.0	K075	1 0 0 0 2	
2.656E+00	5.000E+02	rt	D021	0 0 1 1 2	

2413. $C_{11}H_{12}N_2O_2$

DL-Tryptophan
1H-Indole-3-alanine
DL-α-Amino-3-indolepropionic acid

RN: 54-12-6 **MP** (°C)**:** 289
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	2.083E+00	20	N006	0 0 0 0 0	
1.140E-02	2.328E+00	25	N006	0 0 0 0 0	
1.221E-02	2.494E+00	30	D041	1 0 0 0 1	
1.250E-02	2.553E+00	30	N006	0 0 0 0 0	
1.200E-02	2.451E+00	30	N009	0 0 0 0 0	
1.640E-02	3.349E+00	40	N006	0 0 0 0 0	
1.570E-02	3.206E+00	40	N009	0 0 0 0 0	
2.150E-02	4.391E+00	50	N006	0 0 0 0 0	

2414. $C_{11}H_{12}N_2O_2$

Tryptophan
2-Amino-3-(lH-indol-3-yl)-propanoic acid
3-Indol-3-ylalanine
L-β-3-indolylalanine
Trp
(*S*)-(–)-Tryptophan

RN: 73-22-3 **MP** (°C)**:**
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-02	8.200E+00	0	F300	1 0 0 0 1	
6.042E-02	1.234E+01	20	B032	1 2 2 1 2	
6.395E-02	1.306E+01	22.5	P045	0 0 2 1 2	
6.551E-02	1.338E+01	25	B032	1 2 2 1 2	
5.519E-02	1.127E+01	25	D041	1 0 0 0 2	
5.337E-02	1.090E+01	25	F300	1 0 0 0 2	
6.665E-02	1.361E+01	25	G092	2 1 1 1 1	
6.665E-02	1.361E+01	25	G315	0 0 0 0 0	
5.519E-02	1.127E+01	25	H070	1 0 0 0 2	
6.267E-02	1.280E+01	25.1	N024	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N025	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N026	0 0 0 0 0	
6.665E-02	1.361E+01	25.1	N027	1 1 2 2 2	
1.787E-01	3.650E+01	27	D036	0 0 0 0 0	
5.386E-02	1.100E+01	28	L081	2 1 2 2 2	
7.056E-02	1.441E+01	29.80	B032	1 2 2 1 2	
8.100E-02	1.654E+01	30	N009	0 0 0 0 0	
9.480E-02	1.936E+01	40	N009	0 0 0 0 0	
8.226E-02	1.680E+01	50	F300	1 0 0 0 2	
1.122E-01	2.291E+01	50	N009	0 0 0 0 0	
1.200E-01	2.450E+01	70	F300	1 0 0 0 2	
1.334E-01	2.724E+01	75	D041	1 0 0 0 2	
2.448E-01	5.000E+01	100	F300	1 0 0 0 1	

2415. $C_{11}H_{12}N_2O_2$

5-Ethyl-5-phenylhydantoin
2,4-Imidazolidinedione, 5-ethyl-5-phenyl-
Nirvanol
5-Phenyl-5-ethylhydantoin
Normephenytoin

RN: 631-07-2 **MP** (°C)**:**
MW: 204.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.938E-03	8.044E-01	37	F183	1 0 1 1 1	intrinsic

2416. $C_{11}H_{12}N_2O_4$
Acetamide, *N*-(2-amino-2-oxoethyl)-2-(benzoyloxy)-
RN: 106231-53-2 **MP** (°C)**:** 151.5
MW: 236.23 **BP** (°C)**:** 568.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.175E-02	7.500E+00	22	B427	1 0 0 1 1	in 0.01M HCl
3.175E-02	7.500E+00	22	N317	1 1 2 1 2	

2417. $C_{11}H_{12}N_4O_2S$
2-Sulfanilamido-5-aminopyridine
Benzenesulfonamide, 4-amino-*N*-(5-amino-2-pyridinyl)-
RN: 16840-28-1 **MP** (°C)**:**
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-02	4.180E+00	37	R058	1 2 1 1 2	

2418. $C_{11}H_{12}N_4O_2S$
4-Sulfanilamido-2-methylpyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-methyl-4-pyrimidinyl)-
RN: 599-84-8 **MP** (°C)**:**
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.357E-02	6.230E+00	37	R046	1 2 1 1 2	

2419. $C_{11}H_{12}N_4O_2S$
Sulfamethylpyrimidine
Ulfamerazine
Sulfamerazine
RN: 127-79-7 **MP** (°C)**:** 234
MW: 264.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.967E-04	2.370E-01	20	F073	1 2 2 2 2	
7.641E-04	2.020E-01	20	L058	1 0 1 1 2	
8.012E-04	2.118E-01	25	M440	0 0 0 0 0	
1.400E-03	3.700E-01	37	L091	1 0 0 0 1	pH 5.5
1.203E-03	3.180E-01	37	R045	1 2 1 1 2	
1.381E-03	3.650E-01	37	S192	1 0 1 1 2	pH 6.0
1.551E-03	4.100E-01	38	K006	1 0 0 0 1	

2420. $C_{11}H_{12}N_4O_3S_2$
*N*4-Acetyl sulfamethizole
Acetyl sulfamethylthiazole
RN: 39719-87-4 **MP** (°C)**:**
MW: 312.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-03	4.100E-01	37	B046	1 0 2 2 1	pH 4.5

2421. $C_{11}H_{12}N_4O_3S$
Sulfamethoxypyridazine
Sulphamethoxypyridazine
4-Amino-*N*-(6-methoxy-3-pyridazinyl)-benzenesulfonamide
RN: 80-35-3 **MP** (°C)**:** 182.5
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.067E-03	5.795E-01	25	E314	0 0 0 0 0	intrinsic
2.569E-02	7.200E+00	37	B046	1 0 2 2 2	pH 4.5

2422. $C_{11}H_{12}N_4O_3S$
Sulfameter
Sulphamethoxydiazine
RN: 651-06-9 **MP** (°C)**:** 213
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.700E-01	30	M113	2 2 2 2 0	form III, EFG, 0.1N HCl
2.604E-03	7.300E-01	30	M113	2 2 2 2 0	form II, EFG, 0.1N HCl
1.891E-03	5.300E-01	30	M113	2 2 2 2 0	form I, EFG, 0.1N HCl
2.462E-03	6.900E-01	30	M113	2 2 2 2 0	EFG, 0.1N HCl, amorphous
3.211E-04	9.000E-02	37.5	C081	1 0 1 0 0	EFG, form III
6.243E-04	1.750E-01	37.5	C081	1 0 1 0 0	EFG, form II
4.281E-04	1.200E-01	37.5	C081	1 0 1 0 0	EFG, form I

2423. $C_{11}H_{12}N_4O_3S$
5-Sulfanilamido-2-methoxypyrimidine
Benzenesulfonamide, 4-amino-*N*-(2-methoxy-5-pyrimidinyl)-
RN: 71119-37-4 **MP** (°C)**:**
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.282E-04	9.200E-02	37	R046	1 2 1 1 1	

2424. $C_{11}H_{12}N_4O_3S$
2-Sulfanilamido-4-methoxypyrimidine
Benzenesulfonamide, 4-amino-*N*-(4-methoxy-2-pyrimidinyl)-
RN: 3213-22-7 **MP** (°C)**:**
MW: 280.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.493E-04	1.820E-01	37	R046	1 2 1 1 2	

2425. $C_{11}H_{12}N_4O_5$
2,5-Diacetoxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 2,5-bis[(acetyloxy)methyl]-2,5-dihydro-
RN: 98827-24-8 **MP** (°C)**:** 153–154
MW: 280.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-02	2.900E+00	22	B322	0 0 0 0 0	

2426. $C_{11}H_{12}N_6O_2S$
6-Sulfapurine
RN: **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.447E-05	1.300E-02	20	F073	1 2 2 2 1	

2427. $C_{11}H_{12}O_2$
Cinnamyl acetate
3-Phenylallyl acetate
3-Phenyl-2-propenyl acetate
1-Acetoxy-3-phenyl-2-propene
3-Phenyl-2-propen-1-ol acetate
NSC 46109
RN: 103-54-8 **MP** (°C)**:**
MW: 176.22 **BP** (°C)**:** 170 (°50 torr)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.762E-01	25	D407	1 0 2 2 2	
1.000E-03	1.762E-01	ns	S460	0 0 0 0 0	

2428. $C_{11}H_{12}O_2$
Ethyl cinnamate
Ethyl (E)-cinnamate
Ethyl 3-phenyl propenoate
Ethyl phenylacrylate
RN: 103-36-6 **MP** (°C)**:** 6
MW: 176.22 **BP** (°C)**:** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-03	1.780E-01	25	A002	1 2 1 1 2	

2429. $C_{11}H_{12}O_4$
3,5-Dimethoxycinnamic acid
Predominantly *trans* isomer
RN: 16909-11-8 **MP** (°C)**:** 174.5
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-04	3.144E-02	25	R070	0 0 0 0 0	

2430. $C_{11}H_{12}O_4$
Ethyl acetylsalicylate
Acetyl salicylic acid, ethyl ester
RN: 529-68-0 **MP** (°C)**:**
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.594E-02	3.320E+00	37	G430	0 0 0 0 0	pH 4.5

2431. $C_{11}H_{12}O_4$
Propionyl-*r*-mandelic acid
RN: **MP** (°C)**:** 126
MW: 208.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-02	2.892E+00	0	A043	1 2 1 1 1	
1.389E-02	2.892E+00	0	L035	1 2 2 1 1	
1.675E-02	3.488E+00	10	A043	1 2 1 1 1	
1.675E-02	3.488E+00	10	L035	1 2 2 1 1	
1.770E-02	3.686E+00	15	A043	1 2 1 1 1	
1.770E-02	3.686E+00	15	L035	1 2 2 1 1	
1.818E-02	3.786E+00	20	A043	1 2 1 1 1	
1.818E-02	3.786E+00	20	L035	1 2 2 1 1	
2.484E-02	5.173E+00	25	A043	1 2 1 1 1	

(*continued*)

2431. $C_{11}H_{12}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-02	5.173E+00	25	L035	1 2 2 1 1	
2.817E-02	5.865E+00	30	A043	1 2 1 1 1	
2.817E-02	5.865E+00	30	L035	1 2 2 1 1	
3.528E-02	7.346E+00	35	A043	1 2 1 1 1	
3.528E-02	7.346E+00	35	L035	1 2 2 1 1	
5.789E-02	1.205E+01	40	A043	1 2 1 1 2	
5.789E-02	1.205E+01	40	L035	1 2 2 1 2	
8.724E-02	1.816E+01	45	A043	1 2 1 1 2	
8.724E-02	1.816E+01	45	L035	1 2 2 1 2	
1.606E-01	3.344E+01	50	A043	1 2 1 1 2	
1.606E-01	3.344E+01	50	L035	1 2 2 1 2	

2432. $C_{11}H_{12}O_4S$

Benzoic acid, 2-(acetyloxy)-, (methylthio)methyl ester

RN: 76432-30-9 **MP** (°C)**:**

MW: 240.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.289E-03	5.500E-01	21	N335	0 0 0 0 0	

2433. $C_{11}H_{12}O_5S$

2-(Acetoxy)-benzoic acid, (methylsulfinyl)methyl ester

RN: 76432-33-2 **MP** (°C)**:** 80.5

MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.651E-02	4.230E+00	21	N335	0 0 0 0 0	

2434. $C_{11}H_{12}O_6S$

2-(Acetoxy)-benzoic acid, (methylsulfonyl)methyl ester

RN: 76432-35-4 **MP** (°C)**:** 150

MW: 272.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-04	1.100E-01	21	N335	0 0 0 0 0	

2435. $C_{11}H_{13}ClO_3$
Bexone
4-(2-Methyl-4-chlorophenoxy)butyric acid
4-(MCPB)
MCPB
RN: 94-81-5 **MP** (°C)**:**
MW: 228.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.099E-04	4.800E-02	25	B164	1 0 1 1 1	
1.924E-04	4.400E-02	ns	L024	0 0 0 0 1	
1.924E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.924E-04	4.400E-02	rt	M161	0 0 0 0 1	

2436. $C_{11}H_{13}FN_2O_4$
1-Cyclohexyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, cyclohexyl ester
RN: 109232-74-8 **MP** (°C)**:**
MW: 256.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-03	9.200E-01	22	B332	1 1 0 0 1	pH 4.0

2437. $C_{11}H_{13}F_3N_2O_3S$
Mefluidide
N-(2,4-Dimethyl-5-(((trifluoromethyl)sulfonyl)amino)phenyl)acetamide
Vistar
Embark
MBR 12325
Methafluoridamid
RN: 53780-34-0 **MP** (°C)**:** 184
MW: 310.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.801E-04	1.800E-01	23	M161	1 0 0 0 2	

2438. $C_{11}H_{13}F_3N_4O_4$
Dinitramine
1,3-Benzenediamine, *N*1,*N*1-diethyl-2,6-dinitro-4-(trifluoromethyl)-
*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-*m*-phenylenediamine
*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-phenylenediamine
USB 3584
RN: 29091-05-2 **MP** (°C)**:** 98.5
MW: 322.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.414E-06	1.100E-03	25	M161	1 0 0 0 1	

2439. $C_{11}H_{13}NO$
N,N-Dimethylcinnamide
Cinnamic acid dimethylamide
N,N-Dimethyl-3-phenyl-2-propenamide
RN: 13156-74-6 **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-02	2.926E+00	ns	H350	0 0 0 0 0	

2440. $C_{11}H_{13}NO$
N-Ethylcinnamamide
N-Ethyl-3-phenyl-2-propenamide
RN: 23784-45-4 **MP** (°C)**:**
MW: 175.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.390E-03	1.120E+00	ns	H350	0 0 0 0 0	

2441. $C_{11}H_{13}NO_2S$
2-*p*-Tolyl-4-thiazolidinecarboxylic acid
4-Thiazolidinecarboxylic acid, 2-(4-methylphenyl)-
RN: 67189-37-1 **MP** (°C)**:**
MW: 223.30 **BP** (°C)**:** 444.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.019E-01	21	B414	1 0 0 1 1	very fast and extent decomposition, uncertain value

2442. $C_{11}H_{13}NO_3$
Acetaminophen propionate
Propionic acid, *p*-acetamidophenyl ester
RN: 54942-42-6 **MP** (°C)**:** 130
MW: 207.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-03	3.200E-01	25	B010	1 1 1 1 0	

2443. $C_{11}H_{13}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-ethyl-
2-(Benzoyloxy)-*N*-ethylacetamide
RN: 64649-57-6 **MP** (°C)**:** 106
MW: 207.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.791E-03	1.200E+00	22	B427	1 0 0 1 1	in 0.01M HCl
5.791E-03	1.200E+00	22	N317	1 1 2 1 2	

2444. $C_{11}H_{13}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-dimethyl-
2-(Benzoyloxy)-*N,N*-dimethylacetamide
RN: 106231-54-3 **MP** (°C)**:** 81.5
MW: 207.23 **BP** (°C)**:** 351.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.246E-02	8.800E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.246E-02	8.800E+00	22	N317	1 1 2 1 2	

2445. $C_{11}H_{13}NO_3S$
4-Thiazolidinecarboxylic acid, 2-(4-methoxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(4-methoxyphenyl)-
RN: 65884-40-4 **MP** (°C)**:** 165–166
MW: 239.30 **BP** (°C)**:** 466.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.572E-02	21	B414	1 0 0 1 1	fast decomposition

2446. $C_{11}H_{13}NO_4$
Bendiocarb
2,2-Dimethyl-1,3-benzodioxol-4-ol methylcarbamate
Fuam
Multimet
Garvox
RN: 22781-23-3 **MP** (°C)**:** 129.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.792E-04	4.000E-02	25	M161	1 0 0 0 1	
1.792E-04	4.000E-02	25	W310	1 0 0 0 0	

2447. $C_{11}H_{13}NO_4$
N,N-Dimethyl glycolamide salicylate
2-Hydroxybenzoic acid, 2-(dimethylamino)-2-oxoethyl ester
RN: 114665-08-6 **MP** (°C)**:** 68
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-02	4.400E+00	21	B331	1 2 2 1 0	pH 7.4
1.971E-02	4.400E+00	21	B331	0 0 0 0 0	

2448. $C_{11}H_{13}NO_4$
Ethyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl ethyl ester
Acetanilide, 4′-hydroxy-, ethyl carbonate (ester)
RN: 17243-26-4 **MP** (°C)**:** 121–122
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.928E-03	1.100E+00	37	D029	0 0 0 0 0	

2449. $C_{11}H_{13}NO_4$
Dioxacarb
2-(1,3-Dioxolan-2-yl)phenyl methylcarbamate
2-(1,3-Dioxolan-2-yl)-phenyl *N*-methylcarbamate
Elocron
Famid
RN: 6988-21-2 **MP** (°C)**:** 114.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-02	6.000E+00	20	M161	1 0 0 0 0	

2450. $C_{11}H_{13}NO_4S$
4-Thiazolidinecarboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-
RN: 72678-93-4 **MP** (°C)**:**
MW: 255.29 **BP** (°C)**:** 435.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.532E+00	2.1	B414	1 0 0 1 1	fast decomposition

2451. $C_{11}H_{13}N_3O$

Ampyrone
4-Aminoantipyrine
Aminophenazone

RN: 83-07-8 **MP** (°C)**:** 109
MW: 203.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.053E-01	1.840E+02	5.39	M109	2 1 1 1 0	EFG
1.088E+00	2.211E+02	10.93	M109	2 1 1 1 0	EFG
1.252E+00	2.544E+02	14.20	M109	2 1 1 1 0	EFG
1.527E+00	3.103E+02	20.96	M109	2 1 1 1 0	EFG
2.076E+00	4.218E+02	25.35	M109	2 1 1 1 0	EFG
2.384E+00	4.845E+02	29.87	M109	2 1 1 1 0	EFG
2.400E-01	4.878E+01	30	I010	2 1 2 2 1	EFG, *sic*
2.862E+00	5.816E+02	39.34	M109	2 1 1 1 0	EFG

2452. $C_{11}H_{13}N_3O_3S$

Sulfamoxole
Sulfuno
N-(4,5-Dimethyloxazol-2-yl)sulfanilamide

RN: 729-99-7 **MP** (°C)**:** 193
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-03	9.610E-01	20	K028	2 1 2 1 2	pH 6.0, form I
3.430E-03	9.170E-01	20	K028	2 1 2 1 2	pH 3.8, form I
3.277E-03	8.760E-01	20	K028	2 1 2 1 2	pH 6.0, form II
3.165E-03	8.460E-01	20	K028	2 1 2 1 2	pH 3.8, form II
6.274E-03	1.677E+00	20	K028	2 1 2 1 2	pH 7.3, form I
5.447E-03	1.456E+00	20	K028	2 1 2 1 2	pH 7.3, form II
3.427E-03	9.162E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 205-211 C
3.162E-03	8.453E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 188-195 C

2453. $C_{11}H_{13}N_3O_3S$

Sulfisoxazole
4-Amino-*N*-(3,4-dimethyl-5-isoxazolyl)benzenesulfonamide
3,4-Dimethyl-5-sulfanilamidoisoxazole
Gantrisin
Urogan
Urisoxin

RN: 127-69-5 **MP** (°C)**:** 194
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-03	3.300E-01	37	B046	1 0 2 2 1	pH 4.5
3.142E-04	8.400E-02	37	K022	1 0 1 1 0	intrinsic
1.092E-03	2.920E-01	37	K091	1 0 0 0 2	

2454. $C_{11}H_{13}N_3O_3S$

*N*1-Methyl-*N*1-(5-methyl-3-isoxazolyl)sulfanilamide
*N*1-Methylsulfamethoxazole
RN: 51543-31-8 **MP** (°C)**:**
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-04	1.679E-01	37	K095	2 0 0 0 2	intrinsic

2455. $C_{11}H_{13}N_5O_2$

Carbovir
9-[4α-(Hydroxymethyl)-cyclopent-2-ene-1α-yl]guanine
RN: 118353-05-2 **MP** (°C)**:**
MW: 247.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.015E-03	1.240E+00	25	A338	0 0 0 0 0	

2456. $C_{11}H_{13}N_5O_5$

Arabinosyladenine 5′-formate
Arabinosyladenine 5′-*O*-formate ester
NSC 171240
RN: 55648-40-3 **MP** (°C)**:** 168–170
MW: 295.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-01	3.400E+01	ns	R030	0 0 0 0 0	

2457. $C_{11}H_{14}ClNO$

Propachlor
2-Chloro-*N*-isopropylacetanilide
N-Isopropyl-2-chloroacetanilide
N-Isopropyl-α-chloroacetanilide
RN: 1918-16-7 **MP** (°C)**:** 67
MW: 211.69 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-03	7.000E-01	20	B200	1 0 0 0 2	
3.307E-03	7.000E-01	20	M161	1 0 0 0 2	
3.304E-03	6.995E-01	ns	J008	0 0 0 0 0	
3.304E-03	6.995E-01	ns	M061	0 0 0 0 0	
2.362E-03	5.000E-01	ns	M110	0 0 0 0 0	EFG

2458. $C_{11}H_{14}N_2O$
Cytisine
Cytisin
RN: 485-35-8 **MP** (°C)**:** 155
MW: 190.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.308E+00	4.390E+02	16	F300	1 0 0 0 2	

2459. $C_{11}H_{14}N_2O_3S$
Sulfadicramide
2-Butenamide, *N*-[(4-aminophenyl)sulfonyl]-3-methyl-
N-Sulfanilyl-β,β-dimethylacrylamide
Sulfirgamid
Irgamide
Sulfirgamide

RN: 115-68-4 **MP** (°C)**:** 184.5
MW: 254.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-03	2.610E-01	20	F073	1 2 2 2 2	

2460. $C_{11}H_{14}N_4O_2S_2$
4-Amino-*N*-(5-isopropyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
*N*1-(5-Isopropyl-1,3,4-thiadiazol-2-yl)sulfanilamide
Sulfaisopropylthiadiazole
Glyprothiazole
PASIT
RP 2254
RN: 80-34-2 **MP** (°C)**:**
MW: 298.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.330E-04	2.187E-01	37	A046	2 0 1 1 2	

2461. $C_{11}H_{14}N_4O_2S_2$
4-Amino-*N*-(5-propyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
*N*1-(5-Propyl-1,3,4-thiadiazol-2-yl)sulfanilamide
RN: 71119-32-9 **MP** (°C)**:**
MW: 298.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.980E-04	2.680E-01	37	A046	2 0 1 1 2	

2462. $C_{11}H_{14}N_4O_3$
2-Pivaloyloxymethyl allopurinol
Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-2-yl)methyl ester
RN: 98827-15-7 **MP** (°C)**:** 180–181
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.793E-03	1.700E+00	22	B322	0 0 0 0 0	

2463. $C_{11}H_{14}N_4O_3$
1-Pivaloyloxymethyl allopurinol
Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98827-18-0 **MP** (°C)**:** 185–187
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.078E-03	5.200E-01	22	B322	0 0 0 0 0	

2464. $C_{11}H_{14}N_4O_5$
6-Methoxypurine arabinoside
9H-Purine, 9-β-D-arabinofuranosyl-6-methoxy-
RN: 91969-06-1 **MP** (°C)**:**
MW: 282.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.980E-02	1.406E+01	37	C348	0 0 0 0 0	pH 7.00

2465. $C_{11}H_{14}O$
o-2-Pentenylphenol
Phenol, 2-(2-pentenyl)-
RN: 62536-86-1 **MP** (°C)**:**
MW: 162.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.054E-03	3.332E-01	25	L021	1 0 0 0 0	

2466. $C_{11}H_{14}O_2$
δ-Phenylvaleric acid
Benzenepentanoic acid
5-Phenylvaleric acid
RN: 2270-20-4 **MP** (°C)**:** 59
MW: 178.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.969E-03	1.777E+00	30	D033	2 2 1 2 2	
1.159E-02	2.066E+00	40	D033	2 2 1 2 2	

2467. $C_{11}H_{14}O_2$
4-Butylbenzoic acid
RN: 20651-71-2 **MP** (°C)**:** 100
MW: 178.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-04	1.482E-01	ns	R427	0 0 0 0 0	

2468. $C_{11}H_{14}O_2$
Ethyl hydrocinnamate
Ethyl 3-phenylpropionate
Benzenepropanoic acid, ethyl ester
RN: 2021-28-5 **MP** (°C)**:**
MW: 178.23 **BP** (°C)**:** 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.234E-03	2.200E-01	25	A002	1 2 1 1 1	

2469. $C_{11}H_{14}O_3$
n-Butyl salicylate
2-Hydroxy-benzoic acid, butyl ester
Salicylic acid *n*-butyl ester
Butyl salicylate
Benzoic acid, 2-hydroxy-, butyl ester
RN: 2052-14-4 **MP** (°C)**:**
MW: 194.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	2.800E+00	37	D009	1 2 1 1 1	0.1N HCl

2470. $C_{11}H_{14}O_3$
2-Hydroxy-3-isopropyl-6-methylbenzoic acid
o-Thymotinic acid
RN: 548-51-6 **MP** (°C)**:**
MW: 194.23 **BP** (°C)**:** 316.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.57E-03	>5.00E-01	ns	B404	0 2 1 1 0	

2471. $C_{11}H_{14}O_3$
Butylparaben
Bu-paraben
Butyl 4-hydroxybenzoate
RN: 94-26-8 **MP** (°C)**:** 68.5
MW: 194.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.040E-04	1.367E-01	15	B355	0 0 0 0 0	
8.350E-04	1.622E-01	20	B355	0 0 0 0 0	
1.065E-03	2.069E-01	20	C006	1 2 1 1 2	
1.277E-03	2.481E-01	25	A059	1 0 1 1 1	
1.050E-03	2.039E-01	25	B355	0 0 0 0 0	
8.751E-04	1.700E-01	25	D081	1 2 2 1 2	
1.130E-03	2.195E-01	25	D339	0 0 0 0 0	
5.623E-04	1.092E-01	25	F322	2 0 1 1 0	EFG
1.030E-03	2.000E-01	25	O027	1 0 1 0 0	
7.465E-04	1.450E-01	25	P013	0 0 0 0 0	
1.200E-03	2.331E-01	27	B129	2 2 2 2 1	
1.200E-03	2.331E-01	27	G078	2 1 0 1 0	EFG
1.777E-03	3.452E-01	30	A059	1 0 1 1 1	
2.221E-03	4.314E-01	35	A059	1 0 1 1 1	
2.064E-03	4.009E-01	39.3	G302	2 2 2 2 0	EFG
2.610E-03	5.069E-01	40	A059	1 0 1 1 1	
7.155E-04	1.390E-01	ns	B404	0 2 1 1 0	
1.100E-03	2.137E-01	ns	G067	2 0 1 1 1	
9.989E-04	1.940E-01	rt	I404	0 0 0 0 0	Intrinsic, Average

2472. $C_{11}H_{14}O_3$
4-Methoxyphenylbutyric acid
RN: 4521-28-2 **MP** (°C)**:** 57
MW: 194.23 **BP** (°C)**:** 335

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.122E+00	9.949E+02	37	A407	2 2 2 2 2	

2473. $C_{11}H_{14}O_4$
Dimethyl carbate
Dimelone
RN: 5826-73-3 **MP** (°C)**:** 38
MW: 210.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-02	1.303E+01	35	M061	1 0 0 0 2	

2474. $C_{11}H_{15}BrClO_3PS$
Profenofos
O-(4-Bromo-2-chlorophenyl)-*O*-ethyl-*S*-propyl phosphorothioate
Selecron
Curacron
Polycron
RN: 41198-08-7 **MP** (°C)**:**
MW: 373.64 **BP** (°C)**:** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.353E-05	2.000E-02	20	E048	1 2 1 1 1	
5.353E-05	2.000E-02	20	M161	1 0 0 0 1	
7.499E-05	2.802E-02	ns	S460	0 0 0 0 0	

2475. $C_{11}H_{15}BrN_2O$
Butallylonal
5-(2-Bromoallyl)-5-*sec*-butylbarbituric acid
Dial
RN: 1142-70-7 **MP** (°C)**:** 131.5
MW: 271.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.522E-03	6.840E-01	ns	T003	0 0 0 0 2	

2476. $C_{11}H_{15}FN_2O_4$
1-Hexyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, hexyl ester
RN: 66999-99-3 **MP** (°C)**:** 68
MW: 258.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.808E-03	1.500E+00	22	B332	1 1 0 0 1	pH 4.0

2477. $C_{11}H_{15}NO_2$
m-Isopropylphenyl *N*-methylcarbamate
3-Isopropylphenyl *N*-methylcarbamate
UC-10854
RN: 64-00-6 **MP** (°C)**:** 53
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.398E-04	8.500E-02	30	D089	2 2 0 0 0	
4.398E-04	8.500E-02	30	M061	1 0 0 0 1	

2478. $C_{11}H_{15}NO_2$
Butamben
4-Aminobenzoic acid butyl ester
Butyl *p*-aminobenzoate
RN: 94-25-7 **MP** (°C)**:** 58.0
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	1.990E-01	25	H008	0 0 0 0 0	
8.332E-04	1.610E-01	25	P303	0 0 0 0 0	
1.200E-03	2.319E-01	30	J018	1 2 0 1 1	0.05N NaOH
1.200E-03	2.319E-01	30	J022	1 0 2 1 1	
1.200E-03	2.319E-01	30	N045	1 2 2 2 0	EFG
1.389E-03	2.683E-01	33	P303	0 0 0 0 0	
1.720E-03	3.324E-01	37	F006	1 1 2 2 2	
1.700E-03	3.285E-01	37	J026	2 2 2 1 1	
2.221E-03	4.293E-01	40	P303	0 0 0 0 0	
6.468E-04	1.250E-01	ns	B404	0 2 1 1 0	
7.140E-04	1.380E-01	ns	M066	0 0 0 0 2	
7.140E-04	1.380E-01	rt	B016	0 0 1 1 2	pH 7.4
7.784E-04	1.504E-01	rt	I404	0 0 0 0 0	Average

2479. $C_{11}H_{15}NO_2S$
Ethiofencarb
2-((Ethylthio)methyl)phenyl methylcarbamate
Ethylmercaptomethylphenyl-*N*-methylcarbamate
Ethiophencarp
Croneton
HOX 1901
RN: 29973-13-5 **MP** (°C)**:** <25
MW: 225.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.078E-03	1.820E+00	20	M161	1 0 0 0 2	

2480. $C_{11}H_{15}NO_3$
α,3-*o*-Isopropylidene pyriridoxine
RN: **MP** (°C)**:**
MW: 209.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-02	2.503E+00	37	M067	2 0 1 1 2	

2481. $C_{11}H_{15}NO_3$
Propoxur
o-Isopropoxyphenyl methylcarbamate
Baygon
Blattanex
Blattosep
Suncide
RN: 114-26-1 **MP** (°C)**:** 91
MW: 209.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.301E-03	1.737E+00	10	B324	0 0 0 0 0	
8.316E-03	1.740E+00	10	B324	0 0 0 0 0	
8.885E-03	1.859E+00	20	B300	2 2 1 1 2	
9.244E-03	1.934E+00	20	B324	0 0 0 0 0	
9.206E-03	1.926E+00	20	B324	0 0 0 0 0	
9.558E-03	2.000E+00	20	M161	1 0 0 0 0	
1.166E-02	2.440E+00	30	B324	0 0 0 0 0	
1.163E-02	2.434E+00	30	B324	0 0 0 0 0	
4.732E-02	9.901E+00	ns	M061	0 0 0 0 0	approximate
4.301E-04	9.000E-02	ns	M110	0 0 0 0 0	EFG

2482. $C_{11}H_{15}NO_4$
n-Ethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone
RN: **MP** (°C)**:**
MW: 225.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.908E-01	6.550E+01	20	K050	1 1 1 1 2	

2483. $C_{11}H_{15}N_3O_2$
Formetanate
Methylcarbamic acid, ester with *N′*-(*m*-hydroxyphenyl)-*N,N*-dimethylformamidine
RN: 22259-30-9 **MP** (°C)**:** 102.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E-03	1.000E+00	rt	M161	0 0 0 0 0	

2484. $C_{11}H_{15}N_3O_3$
Orotic acid cyclohexylamide
Orotamide, *N*-cyclohexyl-
RN: 4558-58-1 **MP** (°C)**:** 284–285
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-02	1.779E+01	–4	N018	0 0 0 0 0	
1.100E-01	2.610E+01	16	N018	0 0 0 0 0	
1.330E-01	3.156E+01	25	N018	0 0 0 0 0	

2485. $C_{11}H_{15}N_3O_5$
Triglycidylurazol
Anaxirone
RN: 77658-97-0 **MP** (°C)**:** 91
MW: 269.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.426E-04	2.000E-01	ns	D319	0 0 0 0 0	

2486. $C_{11}H_{15}O_3P$
Diethyl benzoyl phosphonate
Methylene, (diethoxyphosphinyl)phenyl-
RN: 105394-75-0 **MP** (°C)**:**
MW: 226.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<8.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

2487. $C_{11}H_{16}$
tert-Amylbenzene
t-Amylbenzene
RN: 2049-95-8 **MP** (°C)**:** –57.8
MW: 148.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.083E-05	1.050E-02	25	A002	1 2 1 1 2	

2488. $C_{11}H_{16}$
Amylbenzene
n-Pentylbenzene
Pentylbenzene
n-Amylbenzene
n-Pentylbenzene1-phenylpentane
RN: 538-68-1 **MP** (°C)**:** –75
MW: 148.25 **BP** (°C)**:** 205.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-05	3.481E-03	7	O312	2 2 0 2 2	
2.144E-05	3.178E-03	10	O312	2 2 0 2 2	
2.323E-05	3.444E-03	12.5	O312	2 2 0 2 2	
2.153E-05	3.192E-03	15	O312	2 2 0 2 2	
2.311E-05	3.426E-03	17.5	O312	2 2 0 2 2	
2.142E-05	3.176E-03	20	O312	2 2 0 2 2	
2.590E-05	3.840E-03	25	M342	1 0 1 1 2	
2.276E-05	3.374E-03	25	O312	2 2 0 2 2	
2.433E-05	3.607E-03	30	O312	2 2 0 2 2	
2.642E-05	3.917E-03	35	O312	2 2 0 2 2	
2.868E-05	4.252E-03	40	O312	2 2 0 2 2	
3.163E-05	4.689E-03	45	O312	2 2 0 2 2	
6.000E-03	8.895E-01	ns	H307	0 0 0 0 0	

2489. $C_{11}H_{16}$
Pentamethylbenzene
1,2,3,4,5-Pentamethyl benzene
RN: 700-12-9 **MP** (°C)**:** 50.8
MW: 148.25 **BP** (°C)**:** 231.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	1.552E-02	ns	D001	0 0 0 0 2	

2490. $C_{11}H_{16}ClO_2PS_3$
Carbophenothion
O,O-Diethyl *S*-(4-chlorophenylthiomethyl) dithiophosphate
Trithion
Garrathion
Nephocarp
Lethox
RN: 786-19-6 **MP** (°C)**:** <25
MW: 342.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B300	2 1 1 1 2	

(*continued*)

2490. $C_{11}H_{16}ClO_2PS_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.837E-06	6.300E-04	20	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
<1.17E-04	<4.00E-02	ns	M161	0 0 0 0 0	

2491. $C_{11}H_{16}N_2O_2$
4-Aminobenzoic acid-2-(ethyl-amino)ethyl ester
2-(Ethylamino)ethyl 4-aminobenzoate
RN: **MP** (°C)**:**
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-02	5.623E+00	ns	M066	0 0 0 0 1	

2492. $C_{11}H_{16}N_2O_2$
Aminocarb
Phenol, 4-(dimethylamino)-3-methyl, methylcarbamate (ester)
Carbamic acid, methyl-, 4-(dimethylamino)-*m*-tolyl ester
RN: 2032-59-9 **MP** (°C)**:** 93
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.187E-03	8.720E-01	10	B324	0 0 0 0 0	
4.183E-03	8.712E-01	10	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B300	2 2 1 1 2	
4.389E-03	9.142E-01	20	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B324	0 0 0 0 0	
4.393E-03	9.150E-01	20	G300	1 0 0 0 2	
6.521E-03	1.358E+00	30	B324	0 0 0 0 0	
6.540E-03	1.362E+00	30	B324	0 0 0 0 0	

2493. $C_{11}H_{16}N_2O_3$
Vinbarbital
5-Ethyl-5-(1-methyl-1-butenyl)barbituric acid
RN: 125-42-8 **MP** (°C)**:** 161
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-03	7.000E-01	25	B011	2 0 0 1 0	
3.164E-03	7.097E-01	25	B065	1 1 1 1 1	
4.870E-03	1.092E+00	25	V033	2 0 1 1 2	

(*continued*)

2493. $C_{11}H_{16}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.099E+00	25.00	T303	1 0 0 0 1	
7.000E-03	1.570E+00	35.00	T303	1 0 0 0 1	
8.000E-03	1.794E+00	45.00	T303	1 0 0 0 1	

2494. $C_{11}H_{16}N_2O_3$
5-Allyl-5-butylbarbituric acid
n-Butylallylbarbitone
n-Butylallylbarbituric acid
Allylbutylbarbituric acid
Idobutal
RN: 3146-66-5 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.723E-03	1.508E+00	20	J030	1 2 2 2 2	
8.945E-03	2.006E+00	37	J030	1 2 2 2 2	

2495. $C_{11}H_{16}N_2O_3$
Talbutal
Allyl-*sec*-butyl-barbituric acid
5-Allyl-5-*sec*-butylbarbituric acid
RN: 115-44-6 **MP** (°C)**:** 109
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.632E-03	2.160E+00	ns	T003	0 0 0 0 2	

2496. $C_{11}H_{16}N_2O_3$
Butalbital
Itobarbital
5-Allyl-5-isobutylbarbituric acid
Fioricet
Phrenilin
Medigesic
RN: 77-26-9 **MP** (°C)**:** 138
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.590E-03	1.702E+00	25	V033	2 0 1 1 2	
7.600E-03	1.704E+00	25.00	T303	1 0 0 0 1	
1.030E-02	2.310E+00	35.00	T303	1 0 0 0 2	
1.410E-02	3.162E+00	45.00	T303	1 0 0 0 2	

2497. $C_{11}H_{16}N_2O_3$
2,4-Diazaspiro[5.7]tridecane-1,3,5-trione
RN: 143288-62-4 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-03	2.337E-01	25	P350	0 0 0 0 0	intrinsic

2498. $C_{11}H_{16}N_2O_3$
Barbituric acid, 5-ethyl-5-(3-methyl-2-butenyl)
5-Ethyl-5-(3′-methylbut-2′-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)-
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)
5-Ethyl-5-(3-methylbut-2-enyl)barbiturate
RN: 21149-88-2 **MP** (°C)**:**
MW: 224.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.583E-03	1.252E+00	25	P350	0 0 0 0 0	intrinsic

2499. $C_{11}H_{16}N_2O_3S$
Phenbutamide
N-(Phenylsulfonyl)-*N′*-butylurea
N-Benzenesulfonyl-*N′*-*n*-butylurea
RN: 3149-00-6 **MP** (°C)**:** 131
MW: 256.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.995E-04	2.306E-01	37	A028	1 0 2 1 2	intrinsic
9.000E-04	2.307E-01	37	A046	2 0 1 1 2	

2500. $C_{11}H_{16}N_2O_4$
Methyl-2-ethyl-2-allylmalonurate
Methyl 2-ethyl-2-allylmalonurate
RN: 73632-83-4 **MP** (°C)**:** 78.5
MW: 240.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	2.883E+00	23	B152	1 2 1 1 1	pH 3.5

2501. $C_{11}H_{16}N_2O_5$
Methoxycarbonylmethyl-2,2-diethylmalonurate
Methoxycarbonylmethyl 2,2-diethylmalonurate
RN: **MP** (°C)**:** 89
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-03	2.486E+00	23	B152	1 2 1 1 1	pH 3.5

2502. $C_{11}H_{16}N_4O_2$
1-Butyl theobromine
1-Butyl-3,7-dimethylxanthine
1-*n*-Butyl-3,7-dimethylxanthine
RN: 1143-30-2 **MP** (°C)**:** 108
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.370E-02	5.600E+00	30	B042	1 2 1 1 2	

2503. $C_{11}H_{16}N_4O_4$
2,6-Piperazinedione, 4,4′-(1-methyl-1,2-ethanediyl)*bis*-
1,2-Di(4-piperazine-2,6-dione)propane
2,6-Piperazinedione, 4,4′-(1-methyl-1,2-ethanediyl)*bis*-, (±)-, polymer with 1,3-dibromopropane
Propane, 1,3-dibromo-, polymer with (±)-4,4′-(1-methyl-1,2-ethanediyl)bis[2,6-piperazinedione]
RN: 21416-67-1 **MP** (°C)**:** 192 dec
MW: 268.27 **BP** (°C)**:** 233 dec

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-02	3.000E+00	25	P326	0 0 0 0 0	
~5.59E-02	~1.50E+01	25	R017	0 0 0 0 0	enantimer (R)
~1.12E-02	~3.00E+00	25	R017	0 0 0 0 0	

2504. $C_{11}H_{16}O$
p-sec-Amylphenol
4-*sec*-Amylphenol
RN: 25735-67-5 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.408E-04	1.053E-01	25	L021	1 0 0 0 0	

2505. $C_{11}H_{16}O$
p-*n*-Amylphenol
4-*n*-Pentylphenol
RN: 14938-35-3 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.088E-04	9.999E-02	25	L022	1 0 0 0 0	

2506. $C_{11}H_{16}O$
p-*tert*-Pentylphenol
p-(α,α-Dimethylpropyl)phenol
p-(1,1-Dimethylpropyl)phenol
1-Hydroxy-4(2-methyl-2-butyl)benzene
PTAP
RN: 80-46-6 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	
1.023E-03	1.680E-01	25	M127	1 0 0 0 2	

2507. $C_{11}H_{16}O$
4-(1,1-Dimethylethyl)benzenemethanol
4-(1,1-Dimethylethyl)benzyl alcohol
4-*tert*-Butylbenzyl alcohol
4-*tert*-Butylphenylmethanol
p-*tert*-Butylbenzyl alcohol
RN: 877-65-6 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:** 250.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.051E+00	20	B407	1 0 1 2 2	

2508. $C_{11}H_{16}O$
o-*n*-Amylphenol
2-*n*-Amylphenol
RN: 87-26-3 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.365E-04	1.538E-01	25	L022	1 0 0 0 0	

2509. $C_{11}H_{16}O$
o-2-Hexenylphenol
2-2-Hexenylphenol
RN: 75121-79-8 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	

2510. $C_{11}H_{16}O$
2-Methyl-5-*t*-butylphenol
5-*tert*-Butyl-2-methylphenol
5-*tert*-Butyl-*o*-cresol
o-Cresol, 5-*tert*-butyl-
RN: 5781-02-2 **MP** (°C)**:**
MW: 164.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-03	4.160E-01	25	M127	1 0 0 0 2	

2511. $C_{11}H_{16}O_2$
4-*n*-Amyl resorcinol
4-*n*-Amyl-resorcin
RN: 533-24-4 **MP** (°C)**:**
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	2.000E+00	20	F300	1 0 0 0 0	

2512. $C_{11}H_{16}O_2$
3-Pentoxyphenol
m-Pentoxy phenol
Phenol, 3-pentoxy-
RN: 18979-73-2 **MP** (°C)**:**
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-03	3.839E-01	30	B315	0 0 0 0 0	

2513. $C_{11}H_{17}NO_3$
Dimetan
5,5-Dimethyldihydroresorcinyl *N,N*-dimethylcarbamate
RN: 122-15-6 **MP** (°C)**:** 45.5
MW: 211.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	2.913E+01	ns	M061	0 0 0 0 0	approximate

2514. $C_{11}H_{17}N_3O_3$
Orotic acid triethylamide
RN: **MP** (°C)**:** 200–202
MW: 239.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E+00	5.410E+02	25	N018	0 0 0 0 0	

2515. $C_{11}H_{17}N_3O_3S$
Carbutamide
4-Amino-*N*-[(butylamino)carbonyl]-benzenesulfonamide
1-Butyl-3-sulfanilyl urea
RN: 339-43-5 **MP** (°C)**:** 144.5
MW: 271.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.972E-03	5.352E-01	37	A028	1 0 2 1 2	intrinsic
1.950E-03	5.291E-01	37	A046	2 0 1 1 2	
6.634E-03	1.800E+00	37	C054	2 0 2 1 2	0.1N HCl

2516. $C_{11}H_{17}N_3O_6$
Orotic acid triethanolamide
RN: **MP** (°C)**:** 104–108
MW: 287.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E+00	3.778E+02	–4	N018	0 0 0 0 0	
1.882E+00	5.407E+02	16	N018	0 0 0 0 0	
2.187E+00	6.283E+02	25	N018	0 0 0 0 0	

2517. $C_{11}H_{17}O_3PS$
Kitazin
O,O-Diethyl *S*-benzyl thiophosphate
EBP
S-Benzyl *O,O*-di-ethyl phosphorothioate
RN: 13286-32-3 **MP** (°C)**:**
MW: 260.29 **BP** (°C)**:** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	22	K137	1 1 2 1 0	

2518. $C_{11}H_{17}O_3PS_2$
Fensulfothion sulfide
O,O-Diethyl *O*-[*p*-(methylthio)phenyl] phosphorothioate
Phosphorothioic acid, *O,O*-diethyl *O*-[4-(methylthio)phenyl] ester
RN: 3070-15-3 **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E-05	3.700E-03	20	M318	2 2 0 0 2	

2519. $C_{11}H_{17}O_4PS_2$
Fensulfothion
O,O-Diethyl *O*-(4-(methylsulfinyl)phenyl) phosphorothioate
Dasanit
Bay 25141
Agricur
Chemagro 25141
RN: 115-90-2 **MP** (°C)**:** <25
MW: 308.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.473E-03	1.996E+00	20	B169	2 2 1 1 2	
6.473E-03	1.996E+00	20	F318	2 2 0 0 2	
4.994E-03	1.540E+00	25	M161	1 0 0 0 2	

2520. $C_{11}H_{17}O_5PS_2$
Fensulfothion sulfone
Phosphorothioic acid, *O,O*-diethyl *O*-[*p*-(methylsulfonyl)phenyl] ester
Dasanit sulfone
Dasanit sulphone
RN: 14255-72-2 **MP** (°C)**:**
MW: 324.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.242E-04	4.030E-02	10	B324	0 0 0 0 0	
1.243E-04	4.032E-02	10	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	B169	2 2 1 1 2	
2.633E-04	8.540E-02	20	B324	0 0 0 0 0	
2.633E-04	8.539E-02	20	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	M318	2 2 0 0 2	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	

2521. $C_{11}H_{18}N_2O_2S$
Thiopental
5-Ethyl-5-(1-methyl-butyl)-2-thiobarbituric acid
5-Ethyl-5-(1-methylbutyl)-2-thiobarbituric acid
Barbituric acid, 5-ethyl-5-(1-methylbutyl)-2-thio
4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(1-methylbutyl)-2-thioxo
Pentothiobarbital
RN: 76-75-5 **MP** (°C)**:** 158
MW: 242.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.063E-04	5.000E-02	25	A023	1 0 0 1 1	
3.301E-04	8.000E-02	25	B011	2 0 0 1 0	
3.333E-04	8.077E-02	25	B065	1 1 1 1 1	
8.200E-04	1.987E-01	25	G003	1 1 1 1 1	pH 4.7
2.094E-04	5.075E-02	25	P350	0 0 0 0 0	intrinsic
3.000E-04	7.270E-02	30	K108	1 2 2 0 0	
3.301E-04	7.999E-02	35	A023	1 0 0 1 1	
4.126E-04	9.999E-02	40	A023	1 0 0 1 1	

2522. $C_{11}H_{18}N_2O_3$
Amobarbital
5-Ethyl-5-isoamylbarbituric acid
Amylobarbitone
RN: 57-43-2 **MP** (°C)**:** 157
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-03	6.400E-01	20	J030	1 2 2 2 1	
3.533E-03	7.994E-01	25	A023	1 0 0 1 1	
2.475E-03	5.600E-01	25	B011	2 0 0 1 0	
2.665E-03	6.030E-01	25	B065	1 1 1 1 1	
3.900E-03	8.825E-01	25	G003	1 1 1 1 1	pH 4.7
2.170E-03	4.910E-01	25	V033	2 0 1 1 2	
2.200E-03	4.978E-01	25.00	T303	1 0 0 0 1	
3.000E-03	6.788E-01	30	G014	1 1 1 1 0	EFG
3.100E-03	7.015E-01	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
2.846E-03	6.440E-01	30	I015	1 2 2 1 2	pH 6.0, 3 forms
3.200E-03	7.241E-01	30	K108	1 2 2 0 1	
3.300E-03	7.467E-01	35.00	T303	1 0 0 0 1	
4.375E-03	9.900E-01	37	J030	1 2 2 2 1	
4.000E-03	9.051E-01	37	K121	1 2 1 2 0	0.1N HCl
5.517E-03	1.248E+00	40	A023	1 0 0 1 1	
3.820E-02	8.644E+00	40	N008	1 0 1 1 2	*sic*
4.300E-03	9.730E-01	45.00	T303	1 0 0 0 1	
2.342E-03	5.300E-01	ns	T003	0 0 0 0 2	

2523. $C_{11}H_{18}N_2O_3$
Pentobarbital
5-ethyl-5-(1-methyl-butyl)-barbituric acid
RN: 76-74-4 **MP** (°C)**:** 130
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.415E-03	9.990E-01	25	A023	1 0 0 1 1	
2.210E-03	5.000E-01	25	B011	2 0 0 1 0	
2.221E-03	5.026E-01	25	B065	1 1 1 1 1	
3.000E-03	6.788E-01	25	G003	1 1 1 1 1	pH 4.7
4.070E-03	9.210E-01	25	V033	2 0 1 1 2	
4.100E-03	9.277E-01	25.00	T303	1 0 0 0 1	
6.000E-03	1.358E+00	30	K108	1 2 2 0 1	
6.178E-03	1.398E+00	35	A023	1 0 0 1 1	
5.700E-03	1.290E+00	35.00	T303	1 0 0 0 1	
7.000E-03	1.584E+00	37	K121	1 2 1 2 0	0.1N HCl
7.060E-03	1.597E+00	40	A023	1 0 0 1 1	
7.640E-02	1.729E+01	40	N008	1 0 1 1 2	*sic*
6.900E-03	1.561E+00	45.00	T303	1 0 0 0 1	
4.365E-03	9.877E-01	ns	R427	0 0 0 0 0	

2524. $C_{11}H_{18}N_2O_3$
5-*n*-Pentyl-5-ethylbarbituric acid
5-Ethyl-5-pentylbarbituric acid
5-Ethyl-5-pentylbarbiturate
RN: 115-58-2 **MP** (°C)**:** 135.5
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.657E-03	1.506E+00	25	B065	1 2 1 1 1	
2.448E-03	5.540E-01	ns	T003	0 0 0 0 2	

2525. $C_{11}H_{18}N_2O_3$
Pilocarpic acid
1,2-Secopilocarpin-2-oic acid
RN: 28406-15-7 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-04	1.200E-01	23	B340	1 1 2 1 1	pH 9

2526. $C_{11}H_{18}N_4O_2$
Pirimicarb
2-(Dimethylamino)-5,6-dimethyl-4-pyrimidinyl dimethylcarbamate
Abol
Rapid
Fernos
Aphox
RN: 23103-98-2 **MP** (°C)**:** 90.5
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.700E+00	25	M161	1 0 0 0 1	

2527. $C_{11}H_{19}N_3O$
Dimethirimol
2-Dimethylamino-4-hyroxy-5-*n*-butyl-6-methylpyrimidine
RN: 5221-53-4 **MP** (°C)**:** 102
MW: 209.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.734E-03	1.200E+00	25	M161	1 0 0 0 1	
5.727E-03	1.199E+00	ns	M061	0 0 0 0 1	

2528. $C_{11}H_{19}N_3O$
Ethirimol
5-Butyl-2-(ethylamino)-4-hydroxy-6-methylpyrimidine
Milgo
Milcurb super
Milstem
RN: 23947-60-6 **MP** (°C)**:** 159.5
MW: 209.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.556E-04	2.000E-01	rt	M161	0 0 0 0 0	

2529. $C_{11}H_{20}$
2-Methyldecalin
Decahydro-2-methylnaphthalene
RN: 2958-76-1 **MP** (°C)**:**
MW: 152.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-07	4.060E-05	25	B069	1 0 1 1 2	

2530. $C_{11}H_{20}ClN_5$
Chlorazine
2-Chloro-4-diethylamino-6-diethylamino-*s*-triazine
2-Chloro-4,6-*bis*-(diethylamino)-*s*-triazine chlorazine
1,3,5-Triazine
1,3,5-Triazine-2,4-diamine
RN: 580-48-3 **MP** (°C)**:**
MW: 257.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-05	9.000E-03	20	J033	0 0 0 0 0	
3.879E-05	1.000E-02	21	B192	0 0 0 0 1	
3.492E-05	9.000E-03	21	G099	2 0 0 1 0	

2531. $C_{11}H_{20}N_2O_4$
Isopropyl-2,2-diethylmalonurate
Isopropyl 2,2-diethylmalonurate
RN: 73632-77-6 **MP** (°C)**:** 99.5
MW: 244.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	4.153E-01	23	B152	1 2 1 1 1	pH 3.5

2532. $C_{11}H_{20}N_3O_3PS$
Pirimiphos-methyl
Pirimiphosmethyl
RN: 29232-93-7 **MP** (°C)**:** 15
MW: 305.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.139E-05	2.180E-02	10	B324	0 0 0 0 0	
7.946E-05	2.426E-02	10	B324	0 0 0 0 0	
7.363E-05	2.248E-02	20	B300	2 1 1 1 2	
1.119E-04	3.417E-02	20	B324	0 0 0 0 0	
1.005E-04	3.070E-02	20	B324	0 0 0 0 0	
1.640E-04	5.008E-02	30	B324	0 0 0 0 0	
1.474E-04	4.500E-02	30	B324	0 0 0 0 0	
1.638E-05	5.000E-03	30	M161	1 0 0 0 0	*sic*

2533. $C_{11}H_{20}N_6$
1-(Pyrrolidinyl)-3,5-bis(dimethylamino)-*s*-triazine
1-Pyrrolidino-3,5-bis(dimethylamino)-*s*-triazine
RN: 13452-85-2 **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	3.878E-02	25	B386	0 0 0 0 0	

2534. $C_{11}H_{20}N_6O$
1-(Morpholinyl)-3,5-bis(dimethylamino)-*s*-triazine
s-Triazine, 2,4-bis(dimethylamino)-6-morpholino-
RN: 16269-02-6 **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-03	3.288E-01	25	B386	0 0 0 0 0	

2535. $C_{11}H_{20}N_6S$
1-(Thiomorpholinyl)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, *N,N,N′,N′*-tetramethyl-6-(4-thiomorpholinyl)-
RN: 41492-69-7 **MP** (°C)**:**
MW: 268.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.689E-05	1.527E-02	25	B386	0 0 0 0 0	

2536. $C_{11}H_{20}O_2$
Undecylenic acid
10-Undecylenic acid
Hendecenoic acid
RN: 112-38-9 **MP** (°C)**:** 25
MW: 184.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	7.371E-02	30	D051	2 0 0 1 2	
1.074E-04	1.980E-02	30	E005	2 1 1 2 2	
1.248E-04	2.300E-02	40	E005	2 1 1 2 1	
1.411E-04	2.600E-02	50	E005	2 1 1 2 1	
1.000E-03	1.843E-01	60	D051	2 0 0 1 2	
1.736E-04	3.200E-02	60	E005	2 1 1 2 1	

2537. $C_{11}H_{20}O_4$
Hexyl α-acetoxypropionate
Propanoic acid, 2-(acetyloxy)-, hexyl ester
RN: 96884-73-0 **MP** (°C)**:**
MW: 216.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-04	2.000E-01	25	R006	2 2 0 1 1	

2538. $C_{11}H_{20}O_4$
Undecanedioic acid
1,9-Nonanedicarboxylic acid
Nonan-dicarbonsaeure-(1,9)
RN: 1852-04-6 **MP** (°C)**:**
MW: 216.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.358E-02	5.100E+00	21	B040	1 0 1 1 1	*sic*
6.473E-04	1.400E-01	ns	F300	0 0 0 0 2	

2539. $C_{11}H_{20}O_5$
Propanoic acid, 2-[(hexthoxycarbonyl)oxy]-, methyl ester
RN: **MP** (°C)**:**
MW: 232.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.305E-04	9.999E-02	25	R007	0 0 0 0 0	

2540. $C_{11}H_{21}BrO_2$
11-Bromoundecanoic acid
Bromo-11-undecanoique acide
RN: 2834-05-1 **MP** (°C)**:** 49.5
MW: 265.20 **BP** (°C)**:** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.304E-02	30	D051	2 0 0 1 2	
7.500E-04	1.989E-01	60	D051	2 0 0 1 2	

2541. $C_{11}H_{21}NOS$
Cycloate
S-Ethyl *N*-ethylthiocyclohexanecarbamate
RO-Neet
S-Ethyl *N,N*-ethylcyclohexylthiocarbamate
RN: 1134-23-2 **MP** (°C)**:** 12
MW: 215.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.947E-04	8.500E-02	22	B200	1 0 0 0 1	
3.947E-04	8.500E-02	22	F019	1 0 0 0 1	
3.947E-04	8.500E-02	22	M161	1 0 0 0 1	

2542. $C_{11}H_{21}NO_3$
Dipropylaceturethane
RN: **MP** (°C)**:**
MW: 215.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-03	3.998E-01	20	O021	1 2 0 0 0	

2543. $C_{11}H_{21}N_5O$
Ipatone
1,3,5-Triazine, 2-(diethylamino)-4-(isopropylamino)-6-methoxy
1,3,5-Triazine-2,4-diamine, *N,N*-diethyl-6-methoxy-*N′*-(1-methylethyl)
RN: 3004-70-4 **MP** (°C)**:**
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-04	1.000E-01	20	J033	0 0 0 0 0	

2544. $C_{11}H_{21}N_5OS$
Gesaran
2-Methylthio-4-isopropylamino-6-(3-methoxypropylamino)-*s*-triazine
Methoprotryne
RN: 841-06-5 **MP** (°C)**:** 69
MW: 271.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-03	3.200E-01	20	F311	1 2 2 2 1	
1.179E-03	3.200E-01	20	M161	1 0 0 0 2	
1.179E-03	3.200E-01	ns	J033	0 0 0 0 0	
3.681E-03	9.990E-01	ns	M061	0 0 0 0 0	

2545. $C_{11}H_{21}N_5S$
Dimethametryn
N-(1,2-Dimethylpropyl)-*N′*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Belclene 310
RN: 22936-75-0 **MP** (°C)**:**
MW: 255.39 **BP** (°C)**:** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-04	5.000E-02	20	M161	1 0 0 0 1	

2546. $C_{11}H_{21}N_5S$
Dipropetryn
2-(Ethylthio)-4,6-bis(isopropylamino)-*s*-triazine
Cotofor
Sancap
Sancap 80W
RN: 4147-51-7 **MP** (°C)**:** 105
MW: 255.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.600E-02	rt	M161	0 0 0 0 1	

2547. $C_{11}H_{21}N_5S$
Ipatryne
2-Methylmercapto-4-isopropylamino-6-diethylamino-*s*-triazine
RN: **MP** (°C)**:**
MW: 255.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.363E-03	26	G001	1 0 1 1 1	

2548. $C_{11}H_{21}N_7$
1-(1-Piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, *N,N,N′,N′*-tetramethyl-6-(1-piperazinyl)-
RN: 125867-94-9 **MP** (°C)**:**
MW: 251.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-02	2.717E+00	25	B386	0 0 0 0 0	

2549. $C_{11}H_{21}O_5$
Propanoic acid, 2-[(proxycarbonyl)oxy]-, butyl ester
RN: **MP** (°C)**:**
MW: 233.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-04	9.999E-02	25	R007	0 0 0 0 0	

2550. $C_{11}H_{22}N_2O$
Cycluron
N′-Cyclooctyl-*N,N*-dimethylurea
Cyclooctyl-1,1-dimethylurea
OMU
RN: 2163-69-1 **MP** (°C)**:** 138
MW: 198.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.564E-04	1.500E-01	20	B185	0 0 0 0 0	
6.051E-03	1.200E+00	20	G036	1 0 0 0 2	
5.541E-03	1.099E+00	20	M061	1 0 0 0 1	
5.547E-03	1.100E+00	20	M161	1 0 0 0 1	
6.310E-04	1.251E-01	ns	M163	0 0 0 0 0	EFG

2551. $C_{11}H_{22}N_6$
*N*6,*N*6-Diethyl-*N*2,*N*2,*N*4,*N*4-tetramethylmelamine
1,3,5-Triazine-2,4,6-triamine, *N,N*-diethyl-*N′,N′,N″,N″*-tetramethyl-
RN: 16268-75-0 **MP** (°C)**:** 42.0
MW: 238.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-04	7.100E-02	25	C051	1 2 1 1 1	pH 7

2552. $C_{11}H_{22}O_2$

Undecanoic acid
Undecanoique acide

RN: 112-37-8 **MP** (°C)**:** 28.5
MW: 186.30 **BP** (°C)**:** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.382E-03	6.300E-01	0	B136	1 0 2 1 1	
5.744E-04	1.070E-01	20	B136	1 0 2 1 2	
4.992E-04	9.299E-02	20.0	R001	1 1 1 1 1	
6.978E-04	1.300E-01	30	B136	1 0 2 1 2	
2.800E-04	5.216E-02	30	D051	2 0 0 1 2	
5.904E-04	1.100E-01	30.0	R001	1 1 1 1 1	
7.730E-04	1.440E-01	40	B136	1 0 2 1 2	
6.978E-04	1.300E-01	45	B136	1 0 2 1 1	
6.977E-04	1.300E-01	45.0	R001	1 1 1 1 1	
8.052E-04	1.500E-01	60	B136	1 0 2 1 1	
6.000E-04	1.118E-01	60	D051	2 0 0 1 2	
8.050E-04	1.500E-01	60.0	R001	1 1 1 1 1	
3.381E-04	6.300E-02	.0	R001	1 1 1 1 1	

2553. $C_{11}H_{22}O_2$

Methyl caprate
Capric acid methyl ester
Methyl decanoate

RN: 110-42-9 **MP** (°C)**:** –13
MW: 186.30 **BP** (°C)**:** 223

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.36E-05	<4.40E-03	20	M337	2 1 2 2 1	
2.051E-05	3.821E-03	ns	S460	0 0 0 0 0	

2554. $C_{11}H_{22}O_2$

Ethyl nonanoate
Ethyl nonylate

RN: 123-29-5 **MP** (°C)**:**
MW: 186.30 **BP** (°C)**:** 119 at 23 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-04	2.953E-02	ns	S460	0 0 0 0 0	

2555. $C_{11}H_{22}O_2$
3-Hydroxy-2-propyl-5,5-diethyltetrahydrofuran
RN: **MP** (°C)**:**
MW: 186.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2556. $C_{11}H_{22}O_3$
n-Hexyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, hexyl ester
RN: 14144-37-7 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-03	2.999E-01	25	D002	1 2 1 1 0	

2557. $C_{11}H_{22}O_3$
1,3-Dioxolane-4-methanol, 2-hexyl-2-methyl
2-Octanone, cyclic (hydroxymethyl)ethylene acetal
RN: 5660-52-6 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	2.751E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2558. $C_{11}H_{22}O_3$
Octyl lactate
Propanoic acid, 2-hydroxy-, octyl ester
RN: 5464-71-1 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.955E-03	8.000E-01	25	R006	2 2 0 1 0	

2559. $C_{11}H_{22}O_3$
n-Butyl β-*n*-butoxypropionate
Butyl 3-butoxypropionate
Propanoic acid, 3-butoxy-, butyl ester
RN: 14144-48-0 **MP** (°C)**:**
MW: 202.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.951E-03	7.994E-01	25	R034	0 0 0 0 0	

2560. $C_{11}H_{22}O_4$
1,3-Dioxolane-4-methanol, 2-(2-butoxyethyl)-2-methyl
RN: 143458-55-3 **MP** (°C)**:**
MW: 218.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.640E-01	5.763E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2561. $C_{11}H_{23}NOS$
Butylate
S-Ethyl diisobutylthiocarbamate
RN: 2008-41-5 **MP** (°C)**:** <25
MW: 217.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-04	4.500E-02	22	B200	1 0 0 0 1	
2.070E-04	4.500E-02	22	F019	1 0 0 0 1	
1.656E-04	3.599E-02	ns	S460	0 0 0 0 0	
2.070E-04	4.500E-02	rt	M161	0 0 0 0 1	

2562. $C_{11}H_{23}NO_2$
11-Aminoundecanoic acid
Amino-11-undecanoique acide
RN: 2432-99-7 **MP** (°C)**:** 191
MW: 201.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.986E-03	3.998E-01	20	E039	2 0 1 1 1	smoothed
1.600E-03	3.221E-01	30	D051	2 0 0 1 2	
4.962E-03	9.990E-01	30	E039	2 0 1 1 2	smoothed
8.925E-03	1.797E+00	40	E039	2 0 1 1 2	smoothed
1.486E-02	2.991E+00	50	E039	2 0 1 1 2	smoothed
1.000E-02	2.013E+00	60	D051	2 0 0 1 2	
2.471E-02	4.975E+00	60	E039	2 0 1 1 2	smoothed
3.453E-02	6.951E+00	65	E039	2 0 1 1 2	smoothed
4.431E-02	8.920E+00	70	E039	2 0 1 1 2	smoothed
5.405E-02	1.088E+01	75	E039	2 0 1 1 2	smoothed
6.858E-02	1.381E+01	80	E039	2 0 1 1 2	smoothed
8.183E-02	1.647E+01	85	E039	2 0 1 1 2	smoothed
9.740E-02	1.961E+01	90	E039	2 0 1 1 2	smoothed
1.145E-01	2.306E+01	95	E039	2 0 1 1 2	smoothed
1.259E-01	2.534E+01	100	E039	2 0 1 1 2	smoothed

2563. $C_{11}H_{24}$
Undecane
n-Undecane
n-Hendecane
RN: 1120-21-4 **MP** (°C)**:** –26
MW: 156.31 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.60E-06	<1.50E-03	20	M337	2 1 2 2 1	
2.815E-08	4.400E-06	25	M003	1 0 2 2 1	
5.758E-08	9.000E-06	25	T423	0 0 0 0 0	

2564. $C_{12}HCl_7O$
1,2,3,4,6,7,8-Heptachlorodibenzofuran
1,2,3,4,6,7,8-HpCDF
PCDF 131
F 131
RN: 67562-39-4 **MP** (°C)**:** 236
MW: 409.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-12	1.355E-09	22.5	F314	1 1 0 2 2	

2565. $C_{12}HCl_7O_2$
1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin
1,2,3,4,6,7,8-HpCDD
PCDD 73
D 73
Heptachlorodibenzo-*p*-dioxin
RN: 35822-46-9 **MP** (°C)**:** 265
MW: 425.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-12	9.357E-10	7.0	F315	1 2 0 2 2	
2.690E-12	1.144E-09	11.5	F315	1 2 0 2 2	
3.040E-12	1.293E-09	17.0	F315	1 2 0 2 2	
5.400E-12	2.297E-09	21.0	F315	1 2 0 2 2	
6.030E-12	2.565E-09	26.0	F315	1 2 0 2 2	
1.481E-11	6.300E-09	40	F303	1 2 1 2 1	
1.490E-11	6.337E-09	41.0	F315	1 2 0 2 2	

2566. $C_{12}HCl_9$
2,2′,3,3′,4,4′,5,5′,6-Nonachlorobiphenyl
2,3,4,5,6,2′,3′,4′,5′-Nonachlorbiphenyl
RN: 40186-72-9 **MP** (°C)**:** 204.5
MW: 464.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-10	7.800E-08	22	O311	2 2 1 2 1	
5.490E-11	2.549E-08	25	D331	2 1 2 2 2	
5.493E-11	2.550E-08	25	D335	1 0 0 0 2	
2.413E-10	1.120E-07	25	W025	1 0 2 2 2	
5.490E-11	2.549E-08	25.0	M324	1 2 1 1 2	
1.100E-10	5.106E-08	32	D331	2 1 2 2 2	
1.100E-10	5.106E-08	32.0	M324	1 2 1 1 2	
1.420E-10	6.592E-08	40	D331	2 1 2 2 2	
1.420E-10	6.592E-08	40.0	M324	1 2 1 1 2	
2.840E-10	1.318E-07	50	D331	2 1 2 2 2	
2.840E-10	1.318E-07	50.0	M324	1 2 1 1 2	

2567. $C_{12}HCl_9$
2,2′,3,3′,4,5,5′,6,6′-Nonachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,5′,6,6′-nonachloro-
PCB 208
RN: 52663-77-1 **MP** (°C)**:** 182
MW: 464.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.880E-11	1.801E-08	25	M342	1 0 1 1 2	

2568. $C_{12}H_2Br_8$
Octabromobiphenyl
OBBP
Bromkal 80
RN: 27858-07-7 **MP** (°C)**:** 225.0
MW: 785.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.183E-08	2.500E-05	25	N326	1 0 0 0 1	average

2569. $C_{12}H_2Cl_6O$
1,2,3,6,7,8-Hexachlorodibenzofuran
1,2,3,6,7,8-HxCDF
F 121
PCDF 121
2,3,4,7,8,9-Hexachlorodibenzofuran
RN: 57117-44-9 **MP** (°C)**:** 233
MW: 374.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-11	1.769E-08	22.5	F314	1 1 0 2 2	

2570. $C_{12}H_2Cl_6O$
1,2,3,4,7,8-Hexachlorodibenzofuran
1,2,3,4,7,8-HxCDF
F 118
PCDF 118
RN: 70648-26-9 **MP** (°C)**:** 226
MW: 374.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-11	8.247E-09	22.5	F314	1 1 0 2 2	

2571. $C_{12}H_2Cl_6O_2$
1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin
1,2,3,4,7,8-Hexachlorodibenzo[b,e][1,4]dioxin
1,2,3,4,7,8-Hexachlorodibenzo[1,4]dioxin
1,2,3,4,7,8-HxCDD
D 66
PCDD 66
RN: 39227-28-6 **MP** (°C)**:** 273
MW: 390.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.910E-12	2.310E-09	7.0	F315	1 2 0 2 2	
7.980E-12	3.119E-09	11.5	F315	1 2 0 2 2	
1.070E-11	4.182E-09	17.0	F315	1 2 0 2 2	
1.126E-11	4.400E-09	20	F303	1 2 1 2 1	
1.250E-11	4.886E-09	21.0	F315	1 2 0 2 2	
2.020E-11	7.896E-09	26.0	F315	1 2 0 2 2	
4.861E-11	1.900E-08	40	F303	1 2 1 2 2	
4.860E-11	1.900E-08	41.0	F315	1 2 0 2 2	

2572. $C_{12}H_2Cl_8$
2,2′,3,3′,4,4′,5,5′-Octachlorobiphenyl
2,3,4,5,2′,3′,4′,5′-Octachlorbiphenyl
PCB 194
RN: 35694-08-7 **MP** (°C)**:** 156
MW: 429.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.885E-10	1.240E-07	22	O311	2 2 1 2 2	
6.329E-10	2.720E-07	25	W025	1 0 2 2 2	

2573. $C_{12}H_2Cl_8$
2,2′,3,3′,5,5′,6,6′-Octachlorobiphenyl
2,3,5,6,2′,3′,5′,6′-Octachlorbiphenyl
RN: 2136-99-4 **MP** (°C)**:** 161
MW: 429.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.650E-10	1.139E-07	20	D331	2 1 2 2 2	
2.650E-10	1.139E-07	20.0	M324	1 2 1 1 2	
3.420E-10	1.470E-07	25	D331	2 1 2 2 2	
3.420E-10	1.470E-07	25	D335	1 0 0 0 2	
9.150E-10	3.932E-07	25	M342	1 0 1 1 2	
4.188E-10	1.800E-07	25	W025	1 0 2 2 1	
3.420E-10	1.470E-07	25.0	M324	1 2 1 1 2	
4.930E-10	2.119E-07	32	D331	2 1 2 2 2	
4.930E-10	2.119E-07	32.0	M324	1 2 1 1 2	
1.780E-09	7.650E-07	50	D331	2 1 2 2 2	
1.780E-09	7.650E-07	50.0	M324	1 2 1 1 2	

2574. $C_{12}H_3Cl_5O$
2,3,4,7,8-Pentachlorodibenzofuran
2,3,4,7,8-P5CDF
PeCDF, 2,3,4,7,8-
RN: 57117-31-4 **MP** (°C)**:** 195.5
MW: 340.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-10	2.356E-07	22.5	F314	1 1 0 2 2	

2575. $C_{12}H_3Cl_5O_2$
1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin
Dibenzo[b,e][1,4]dioxin, 1,2,3,4,7-pentachloro-
PCDD 50
RN: 39227-61-7 **MP** (°C)**:** 195
MW: 356.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-10	5.061E-08	7.0	F315	1 2 0 2 2	
1.880E-10	6.701E-08	11.5	F315	1 2 0 2 2	
2.440E-10	8.697E-08	17.0	F315	1 2 0 2 2	
3.367E-10	1.200E-07	20	F303	1 2 1 2 1	
3.450E-10	1.230E-07	21.0	F315	1 2 0 2 2	
4.630E-10	1.650E-07	26.0	F315	1 2 0 2 2	
1.291E-09	4.600E-07	40	F303	1 2 1 2 1	
1.280E-09	4.562E-07	41.0	F315	1 2 0 2 2	

2576. $C_{12}H_3Cl_7$
2,2′,3,3′,4,4′,5-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,4′,5-heptachloro-
PCB 170
CB 170
RN: 35065-30-6 **MP** (°C)**:** 134.5
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.778E-09	3.470E-06	20	M336	2 0 2 2 2	

2577. $C_{12}H_3Cl_7$
2,2′,3,4′,5,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5,5′,6-heptachloro-
PCB 187
RN: 52663-68-0 **MP** (°C)**:** 104
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-08	4.510E-06	20	M336	2 0 2 2 2	

2578. $C_{12}H_3Cl_7$
2,2′,3,3′,5,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5,5′,6-heptachloro-
PCB 178
RN: 52663-67-9 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.840E-06	20	M336	2 0 2 2 2	

2579. $C_{12}H_3Cl_7$
2,2′,3,3′,4,6,6′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,6,6′-heptachloro-
PCB 176
RN: 52663-65-7 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-08	5.850E-06	20	M336	2 0 2 2 2	

2580. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,6-heptachloro-
PCB 173
RN: 68194-16-1 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.052E-08	4.160E-06	20	M336	2 0 2 2 2	

2581. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,6′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,6′-heptachloro-
PCB 174
RN: 38411-25-5 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-08	5.250E-06	20	M336	2 0 2 2 2	

2582. $C_{12}H_3Cl_7$
2,2′,3,4,4′,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5′,6-heptachloro-
PCB 183
RN: 52663-69-1 **MP** (°C)**:** 83
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-08	4.900E-06	20	M336	2 0 2 2 2	

2583. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5′,6-heptachloro-
PCB 175
RN: 40186-70-7 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E-08	8.940E-06	20	M336	2 0 2 2 2	

2584. $C_{12}H_3Cl_7$
2,2′,3,3′,4,4′,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,4′,6-heptachloro-
PCB 171
RN: 52663-71-5 **MP** (°C)**:** 117
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-08	4.120E-06	20	M336	2 0 2 2 2	
5.490E-09	2.170E-06	25	M342	1 0 1 1 2	
5.490E-09	2.170E-06	ns	M308	0 0 1 1 2	

2585. $C_{12}H_3Cl_7$
2,2′,3,3′,4′,5,6-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5′,6′-heptachloro-
PCB 177
RN: 52663-70-4 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.219E-08	4.820E-06	20	M336	2 0 2 2 2	

2586. $C_{12}H_3Cl_7$
2,2′,3,3′,4,5,5′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4,5,5′-heptachloro-
PCB 172
RN: 52663-74-8 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-08	4.300E-06	20	M336	2 0 2 2 2	

2587. $C_{12}H_3Cl_7$
2,2′,3,4,4′,5,5′-Heptachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5,5′-heptachloro-
PCB 180
RN: 35065-29-3 **MP** (°C)**:** 112
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.739E-09	3.850E-06	20	M336	2 0 2 2 2	

2588. $C_{12}H_3Cl_7$
Heptachlorobiphenyl
1,1′-Biphenyl, heptachloro-
Heptachlorodiphenyl
RN: 28655-71-2 **MP** (°C)**:**
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-08	6.250E-06	11.5	D085	0 0 0 0 0	mixed isomers

2589. $C_{12}H_3Cl_7$
2,2′,3,4,5,5′,6-Heptachlorobiphenyl
2,3,4,5,6,2′,5′-Heptachlorbiphenyl
PCB 185
RN: 52712-05-7 **MP** (°C)**:** 147
MW: 395.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-08	5.460E-06	20	M336	2 0 2 2 2	*sic*
1.189E-09	4.700E-07	25	W025	1 0 2 2 1	

2590. $C_{12}H_4Br_6$
FireMaster FF-1 (hexabromobiphenyl mixture)
RN: **MP** (°C)**:**
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2591. $C_{12}H_4Br_6$
2,2′,4,4′,6,6′-Hexabromobiphenyl
Hexabromobiphenyl
Polybromilated biphenyl
RN: 36355-01-8 **MP** (°C)**:** 72
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.954E-04	6.247E-01	26.5	G312	0 0 0 0 0	

2592. $C_{12}H_4Br_6$
Fire Master BP-6 (hexabromophenyl mixture)
RN: 59536-65-1 **MP** (°C)**:**
MW: 627.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2593. $C_{12}H_4Br_6O$
2,2′,4,4′,5,5′-Hexabromodiphenylether
RN: **MP** (°C)**:**
MW: 643.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.723E-11	3.040E-08	10	K431	0 0 0 0 0	
7.831E-11	5.040E-08	25	K431	0 0 0 0 0	
1.896E-10	1.220E-07	35	K431	0 0 0 0 0	

2594. $C_{12}H_4Cl_4O$
2,3,7,8-Tetrachlorodibenzofuran
2,3,7,8-T4CDF
RN: 51207-31-9 **MP** (°C)**:** 227
MW: 305.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-09	4.192E-07	22.5	F314	1 1 0 2 2	

2595. $C_{12}H_4Cl_4O_2$

1,2,3,4-Tetrachlorodibenzo-*p*-dioxin
1,2,3,4-TCDD
1,2,3,4-Tetrachlorodibenzo[b,e][1,4]dioxin
RN: 30746-58-8 **MP** (°C)**:** 184–186
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-10	1.130E-07	4.0	D330	2 2 1 2 2	
4.007E-11	1.290E-08	4.3	L321	2 0 2 2 2	
1.065E-09	3.430E-07	5	S352	2 2 0 2 2	
1.401E-09	4.510E-07	15	S352	2 2 0 2 2	
1.500E-09	4.830E-07	17.3	L321	2 0 2 2 2	
1.708E-09	5.500E-07	25	S352	2 2 0 2 1	average of 2
1.957E-09	6.300E-07	25	S352	2 2 0 2 1	
1.460E-09	4.701E-07	25.0	D330	2 2 1 2 2	
3.541E-09	1.140E-06	35	S352	2 2 0 2 2	
3.630E-09	1.169E-06	40.0	D330	2 2 1 2 2	
6.476E-09	2.085E-06	45	S352	2 2 0 2 2	

2596. $C_{12}H_4Cl_4O_2$

2,3,7,8-Tetrachlorodibenzo-*p*-dioxin
TCDD
2,3,7,8-Tetrachlorodibenzodioxin
RN: 1746-01-6 **MP** (°C)**:** 310
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-11	1.930E-08	22	M340	1 2 2 1 2	
6.212E-10	2.000E-07	ns	C098	0 0 0 0 0	
6.212E-10	2.000E-07	ns	K138	0 0 0 0 2	
6.212E-10	2.000E-07	ns	N320	0 0 0 0 0	
2.457E-11	7.910E-09	rt	A323	0 2 2 1 2	

2597. $C_{12}H_4Cl_4O_2$

1,3,6,8-Tetrachlorodibenzo-*p*-dioxin
PCDD 42
1,3,6,8-Tetrachlorodibenzo[1,4]dioxin
RN: 33423-92-6 **MP** (°C)**:** 219
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.939E-10	3.200E-07	20	F303	1 2 1 2 1	
9.939E-10	3.200E-07	20	W319	1 2 1 2 1	
1.211E-09	3.900E-07	40	F303	1 2 1 2 1	
1.211E-09	3.900E-07	40	W319	1 2 1 2 1	
9.845E-10	3.170E-07	ns	W332	0 1 0 2 2	

2598. $C_{12}H_4Cl_4O_2$
1,2,3,7-Tetrachlorodibenzo-*p*-dioxin
PCDD 29
RN: 67028-18-6 **MP** (°C)**:** 175
MW: 321.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.560E-10	2.434E-07	7.0	F315	1 2 0 2 2	
8.120E-10	2.614E-07	11.5	F315	1 2 0 2 2	
1.250E-09	4.025E-07	17.0	F315	1 2 0 2 2	
1.336E-09	4.300E-07	20	F303	1 2 1 2 1	
1.490E-09	4.797E-07	21.0	F315	1 2 0 2 2	
2.260E-09	7.277E-07	26.0	F315	1 2 0 2 2	
3.944E-09	1.270E-06	40	F303	1 2 1 2 1	
4.330E-09	1.394E-06	41.0	F315	1 2 0 2 2	

2599. $C_{12}H_4Cl_6$
2,2′,3,4′,5,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5,5′-hexachloro-
PCB 146
RN: 51908-16-8 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.103E-08	7.590E-06	20	M336	2 0 2 2 2	

2600. $C_{12}H_4Cl_6$
2,2′,3,3′,4,4′-Hexachlorobiphenyl
2,3,4,2′,3′,4′-Hexachlorbiphenyl
PCB 128
1,1′-Biphenyl, 2,2′,3,3′,4,4′-hexachloro-
RN: 38380-07-3 **MP** (°C)**:** 150
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-08	6.700E-06	20	M336	2 0 2 2 2	*sic*
9.690E-10	3.497E-07	25	D306	2 1 2 2 2	
7.840E-10	2.829E-07	25	M342	1 0 1 1 2	
1.219E-09	4.400E-07	25	W025	1 0 2 2 1	

2601. $C_{12}H_4Cl_6$
2,2′,3,3′,4,5-Hexachlorobiphenyl
2,3,4,5,2′,3′-Hexachlorbiphenyl
2,2′,3,3′,4,5′-Hexachlorobiphenyl
PCB 129
RN: 55215-18-4 **MP** (°C)**:** 101
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-08	5.690E-06	20	M336	2 0 2 2 2	
1.610E-08	5.810E-06	25	D306	2 1 2 2 2	
2.355E-09	8.500E-07	25	W025	1 0 2 2 1	

2602. $C_{12}H_4Cl_6$
2,3,3′,4,4′,5′-Hexachlorobiphenyl
2,3,3′,4,4′,5-Hexachlorobiphenyl
RN: 38380-08-4 **MP** (°C)**:** 127
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-08	5.330E-06	20	M336	2 0 2 2 2	

2603. $C_{12}H_4Cl_6$
2,2′,3,3′,6,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,6,6′-hexachloro-, (+)-
(+)-PCB 136
RN: 207004-30-6 **MP** (°C)**:** 114
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.050E-09	1.101E-06	4	D331	2 1 2 2 2	
3.050E-09	1.101E-06	4.0	M324	1 2 1 1 2	
9.010E-09	3.252E-06	20	D331	2 1 2 2 2	
5.586E-08	2.016E-05	20	M336	2 0 2 2 2	
9.010E-09	3.252E-06	20.0	M324	1 2 1 1 2	
1.250E-08	4.511E-06	25	D331	2 1 2 2 2	
1.250E-08	4.510E-06	25	D335	1 0 0 0 2	
1.670E-08	6.027E-06	25	M342	1 0 1 1 2	
1.250E-08	4.511E-06	25.0	M324	1 2 1 1 2	
1.850E-08	6.676E-06	32	D331	2 1 2 2 2	
1.850E-08	6.676E-06	32.0	M324	1 2 1 1 2	
1.670E-08	6.027E-06	ns	M308	0 0 1 1 2	

2604. $C_{12}H_4Cl_6$
2,2′,3,3′,5,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5,6′-hexachloro-
PCB 135
RN: 52744-13-5 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2605. $C_{12}H_4Cl_6$
2,3,3′,4′,5,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5,6-hexachloro-
PCB 163
RN: 74472-44-9 **MP** (°C)**:** 122
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-08	5.300E-06	25	B319	2 0 1 2 1	
1.471E-08	5.310E-06	25	H341	1 0 0 0 2	

2606. $C_{12}H_4Cl_6$
2,3,3′,4,4′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4,4′,6-hexachloro-
PCB 158
RN: 74472-42-7 **MP** (°C)**:** 107
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.070E-06	20	M336	2 0 2 2 2	

2607. $C_{12}H_4Cl_6$
Hexachlorobiphenyl
1,1′-Biphenyl, hexachloro-
RN: 26601-64-9 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.754E-08	9.940E-06	11.5	D085	0 0 0 0 0	mixed isomers

2608. $C_{12}H_4Cl_6$
Aroclor 1260
Arochlor 1260
RN: 11096-82-5 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:** 402.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.879E-08	1.400E-05	4	M336	2 0 2 2 1	
3.990E-08	1.440E-05	20	M336	2 0 2 2 2	
6.927E-08	2.500E-05	20	N326	1 0 0 0 1	

2609. $C_{12}H_4Cl_6$
2,2′,3,5,5′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5,5′,6-hexachloro-
PCB 151
RN: 52663-63-5 **MP** (°C)**:** 100
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-08	1.355E-05	20	M336	2 0 2 2 2	

2610. $C_{12}H_4Cl_6$
2,2′,3,3′,4,6-Hexachlorobiphenyl
2,2′,3,4′,5′,6′-Hexachlorobiphenyl
PCB 131
RN: 61798-70-7 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.358E-08	1.212E-05	20	M336	2 0 2 2 2	

2611. $C_{12}H_4Cl_6$
2,2′,3,3′,5,6-Hexachlorobiphenyl
2,3,5,6,2′,3′-Hexachlorbiphenyl
RN: 52704-70-8 **MP** (°C)**:** 132
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-08	1.295E-05	20	M336	2 0 2 2 2	*sic*
2.522E-09	9.100E-07	25	W025	1 0 2 2 1	

2612. $C_{12}H_4Cl_6$
2,2′,3,4,5,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,5,5′-hexachloro-
PCB 141
RN: 52712-04-6 **MP** (°C)**:** 85
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.092E-08	7.550E-06	20	M336	2 0 2 2 2	

2613. $C_{12}H_4Cl_6$
2,2′,3,4,5′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,5′,6-hexachloro-
PCB 144
RN: 68194-14-9 **MP** (°C)**:**
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2614. $C_{12}H_4Cl_6$
2,2′,4,4′,5,5′-Hexachlorobiphenyl
2,4,5,2′,4′,5′-PCB
2,4,5,2′,4′,5′-Hexachlorobiphenyl
PCB 129
PCB 153
RN: 35065-27-1 **MP** (°C)**:** 103
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-08	4.619E-06	4.0	D330	2 2 1 2 2	
2.533E-08	9.140E-06	20	M336	2 0 2 2 2	*sic*
7.759E-09	2.800E-06	22	C413	2 0 2 2 1	
3.187E-09	1.150E-06	22	O311	2 2 1 2 2	
2.632E-09	9.500E-07	24	C053	0 0 0 0 0	
2.632E-09	9.500E-07	24	F071	1 1 2 1 1	
2.632E-09	9.500E-07	24	M344	1 0 0 0 1	
2.390E-09	8.625E-07	25	D306	2 1 2 2 2	
3.325E-09	1.200E-06	25	W025	1 0 2 2 1	
2.340E-08	8.445E-06	25.0	D330	2 2 1 2 2	
3.540E-08	1.278E-05	40	D330	2 2 1 2 2	
2.641E-09	9.530E-07	ns	H058	0 1 2 1 2	

2615. $C_{12}H_4Cl_6$
2,2′,3,4,4′,5′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5′-hexachloro-
PCB 138
CB 138
K 138
RN: 35065-28-2 **MP** (°C)**:** 80.5
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.020E-08	7.290E-06	20	M336	2 0 2 2 2	

2616. $C_{12}H_4Cl_6$
2,2′,3,4,4′,6-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,6-hexachloro-
PCB 139
RN: 56030-56-9 **MP** (°C)**:** 73
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.372E-08	1.217E-05	20	M336	2 0 2 2 2	

2617. $C_{12}H_4Cl_6$
2,2′,3,4,4′,5-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′,5-hexachloro-
PCB 137
RN: 35694-06-5 **MP** (°C)**:** 77
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-08	8.400E-06	20	M336	2 0 2 2 2	

2618. $C_{12}H_4Cl_6$
2,2′,4,4′,6,6′-Hexachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′,6,6′-hexachloro-
PCB 155
RN: 33979-03-2 **MP** (°C)**:** 112.5
MW: 360.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-09	1.090E-06	22	O311	2 2 1 2 2	
6.280E-09	2.266E-06	25	D306	2 1 2 2 2	
9.120E-09	3.291E-06	25	L322	1 1 2 2 2	
1.130E-09	4.078E-07	25	M342	1 0 1 1 2	
2.494E-09	9.000E-07	25	W025	1 0 2 2 1	
1.130E-09	4.078E-07	ns	M308	0 0 1 1 2	

2619. $C_{12}H_5Br_5$
2,2′,4,5,5′-Pentabromobiphenyl
1,1′-Biphenyl, 2,2′,4,5,5′-pentabromo-
PBB 101
RN: 67888-96-4 **MP** (°C)**:**
MW: 548.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-10	1.032E-07	4.0	D330	2 2 1 2 2	
8.060E-10	4.423E-07	25	D330	2 2 1 2 2	
1.790E-09	9.822E-07	40.0	D330	2 2 1 2 2	

2620. $C_{12}H_5Br_5O$
2,2′,4,4′,5-Pentabromodiphenyl ether
RN: **MP** (°C)**:**
MW: 564.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.108E-09	2.320E-06	10	K431	0 0 0 0 0	
7.738E-09	4.370E-06	25	K431	0 0 0 0 0	
1.186E-08	6.700E-06	35	K431	0 0 0 0 0	

2621. $C_{12}H_5Cl_3O_2$
1,2,4-Trichlorodibenzo-*p*-dioxin
Dibenzo[b,e][1,4]dioxin, 1,2,4-trichloro-
PCDD 14
RN: 39227-58-2 **MP** (°C)**:** 129
MW: 287.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.617E-09	2.190E-06	5	S352	2 2 0 2 2	
1.659E-08	4.770E-06	15	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
5.801E-08	1.668E-05	35	S352	2 2 0 2 2	
9.815E-08	2.822E-05	45	S352	2 2 0 2 2	

2622. $C_{12}H_5Cl_5$
2,2′,3,4,4′-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4,4′-pentachloro-
PCB 85
RN: 65510-45-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.712E-08	2.191E-05	20	M336	2 0 2 2 2	

2623. $C_{12}H_5Cl_5$
2,2′,3,4′,6-Pentachlorobiphenyl
2,2′,4,6,6′-Pentachlorobiphenyl
PCB 104
RN: 56558-16-8 **MP** (°C)**:** 85
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-07	3.945E-05	20	M336	2 0 2 2 2	
4.770E-08	1.557E-05	25	D306	2 1 2 2 2	

2624. $C_{12}H_5Cl_5$
2,2′,3,3′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,6-pentachloro-
PCB 84
RN: 52663-60-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-07	4.702E-05	20	M336	2 0 2 2 2	

2625. $C_{12}H_5Cl_5$
2,2′,3,3′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,5-pentachloro-
PCB 83
RN: 60145-20-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.648E-08	2.823E-05	20	M336	2 0 2 2 2	

2626. $C_{12}H_5Cl_5$
2′,3,4,5,5′-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5,5′-pentachloro-
PCB 124
RN: 70424-70-3 **MP** (°C)**:** 105
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-08	1.581E-05	20	M336	2 0 2 2 2	

2627. $C_{12}H_5Cl_5$
2,2′,3′,4,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′,5′-pentachloro-
PCB 87
RN: 41464-51-1 **MP** (°C)**:** 81
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.703E-08	2.841E-05	20	M336	2 0 2 2 2	

2628. $C_{12}H_5Cl_5$
2,2′,3,4,5′-Pentachlorobiphenyl
2,3,4,2′,5′-Pentachlorbiphenyl
PCB 87
RN: 38380-02-8 **MP** (°C)**:** 112
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.009E-08	2.941E-05	20	M336	2 0 2 2 2	
1.379E-08	4.500E-06	25	W025	1 0 2 2 1	

2629. $C_{12}H_5Cl_5$
2,3,3′,4′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,6-pentachloro-
PCB 110
RN: 38380-03-9 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.829E-08	2.882E-05	20	M336	2 0 2 2 2	

2630. $C_{12}H_5Cl_5$
2′,3,3′,4,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5′-pentachloro-
PCB 122
RN: 76842-07-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.933E-08	1.284E-05	20	M336	2 0 2 2 2	

2631. $C_{12}H_5Cl_5$
2,2′,3,3′,4-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′,4-pentachloro-
PCB 82
RN: 52663-62-4 **MP** (°C)**:** 119
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.908E-08	2.908E-05	20	M336	2 0 2 2 2	

2632. $C_{12}H_5Cl_5$
2,2′,3,4,5-Pentachlorobiphenyl
2,3,4,5,2′-Pentachlorbiphenyl
PCB 86
RN: 55312-69-1 **MP** (°C)**:** 112
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.046E-08	2.300E-05	23	W024	0 0 0 0 0	
1.042E-07	3.400E-05	25	B319	2 0 1 2 1	
1.069E-07	3.490E-05	25	H341	1 0 0 0 2	
3.002E-08	9.800E-06	25	W025	1 0 2 2 2	

2633. $C_{12}H_5Cl_5$
2,2′,3,4,6-Pentachlorobiphenyl
2,3,4,6,2′-Pentachlorbiphenyl
PCB 88
RN: 55215-17-3 **MP** (°C)**:** 63
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.676E-08	1.200E-05	25	W025	1 0 2 2 2	

2634. $C_{12}H_5Cl_5$
2,2′,3,5′,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5′,6-pentachloro-
PCB 95
RN: 38379-99-6 **MP** (°C)**:** 94
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-07	5.413E-05	20	M336	2 0 2 2 2	

2635. $C_{12}H_5Cl_5$
2,2′,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′,5-pentachloro-
PCB 99
RN: 38380-01-7 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.798E-08	2.219E-05	20	M336	2 0 2 2 2	

2636. $C_{12}H_5Cl_5$
2,3′,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,4′,5-pentachloro-
PCB 118
CB 118
RN: 31508-00-6 **MP** (°C)**:** 109
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.117E-08	1.344E-05	20	M336	2 0 2 2 2	

2637. $C_{12}H_5Cl_5$
2,3,3′,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′,5-pentachloro-
PCB 107
RN: 70424-68-9 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.546E-08	1.484E-05	20	M336	2 0 2 2 2	

2638. $C_{12}H_5Cl_5$
2,3,4,4′,5-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,4,4′,5-pentachloro-
PCB 114
RN: 74472-37-0 **MP** (°C)**:** 98
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-08	1.598E-05	20	M336	2 0 2 2 2	

2639. $C_{12}H_5Cl_5$
2,3,4,5,6-Pentachlorobiphenyl
1,1′-Biphenyl, 2,3,4,5,6-pentachloro-
PCB 116
RN: 18259-05-7 **MP** (°C)**:** 123
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.166E-08	1.360E-05	22	O311	2 2 1 2 2	
1.230E-08	4.015E-06	25	D306	2 1 2 2 2	
1.680E-08	5.484E-06	25	M342	1 0 1 1 2	
2.083E-08	6.800E-06	25	W025	1 0 2 2 1	
1.680E-08	5.484E-06	ns	M308	0 0 1 1 2	

2640. $C_{12}H_5Cl_5$
2,2′,4,5,5′-Pentachlorobiphenyl
2,4,5,2′,5′-PCB
2,2′,4,5,5′-PCB
RN: 37680-73-2 **MP** (°C)**:** 77
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-08	6.137E-06	4	D331	2 1 2 2 2	
1.880E-08	6.137E-06	4.0	M324	1 2 1 1 2	
3.710E-08	1.211E-05	20	D331	2 1 2 2 2	
8.044E-08	2.626E-05	20	M336	2 0 2 2 2	
3.710E-08	1.211E-05	20.0	M324	1 2 1 1 2	
3.063E-08	1.000E-05	24	C053	0 0 0 0 0	
3.370E-08	1.100E-05	24	C311	0 0 0 0 0	EFG
3.063E-08	1.000E-05	24	F071	1 1 2 1 1	
3.063E-08	1.000E-05	24	M344	1 0 0 0 1	
3.370E-08	1.100E-05	25	C313	0 0 0 0 0	
2.070E-08	6.757E-06	25	D306	2 1 2 2 2	
4.720E-08	1.541E-05	25	D331	2 1 2 2 2	
4.718E-08	1.540E-05	25	D335	1 0 0 0 2	
5.920E-08	1.933E-05	25	M342	1 0 1 1 2	
1.287E-08	4.200E-06	25	W025	1 0 2 2 1	
4.720E-08	1.541E-05	25.0	M324	1 2 1 1 2	
6.830E-08	2.230E-05	32	D331	2 1 2 2 2	
6.830E-08	2.230E-05	32.0	M324	1 2 1 1 2	
3.155E-08	1.030E-05	ns	H058	0 1 2 1 2	
5.820E-08	1.900E-05	ns	M118	0 1 1 1 1	
5.920E-08	1.933E-05	ns	M308	0 0 1 1 2	

2641. $C_{12}H_5Cl_5$
Pentachlorobiphenyl
2,2′,4,4′,6-Pentachlorobiphenyl
Kanekrol 500
RN: 25429-29-2 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.341E-08	2.070E-05	11.5	D085	0 0 0 0 0	mixed isomers
9.496E-08	3.100E-05	22.5	G301	0 0 0 0 0	

2642. $C_{12}H_5N_5O_{11}$
Pentanitrophenylether
Benzene, 2-(2,4-dinitrophenoxy)-1,3,5-trinitro-
RN: 5950-87-8 **MP** (°C)**:**
MW: 395.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.771E-04	7.000E-02	27	D067	1 2 0 0 0	
4.302E-04	1.700E-01	50	D067	1 2 0 0 1	
2.404E-03	9.500E-01	100	D067	1 2 0 0 1	

2643. $C_{12}H_5N_7O_{12}$
Hexanitrodiphenylamine
Benzenamine, 2,4,6-trinitro-*N*-(2,4,6-trinitrophenyl)-
RN: 131-73-7 **MP** (°C)**:**
MW: 439.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E-04	6.000E-02	17	D070	1 2 0 0 0	
4.325E-04	1.900E-01	50	D070	1 2 0 0 1	
7.738E-04	3.399E-01	100	D070	1 2 0 0 1	

2644. $C_{12}H_6Br_4$
2,2′,5,5′-Tetrabromobiphenyl
Tetrabromobiphenyl
RN: 59080-37-4 **MP** (°C)**:** 143
MW: 469.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-03	4.054E+00	26.5	G312	0 0 0 0 0	

2645. $C_{12}H_6Br_4O$
2,2′,4,4′-Tetrabromodiphenylether
RN: **MP** (°C)**:**
MW: 485.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.661E-08	8.070E-06	10	K431	0 0 0 0 0	
3.026E-08	1.470E-05	25	K431	0 0 0 0 0	
5.105E-09	2.480E-06	35	K431	0 0 0 0 0	

2646. $C_{12}H_6Cl_2O_2$
2,7-Dichlorodibenzo-*p*-dioxin
2,7-DCDD
2,8-Dichlorodibenzodioxin
RN: 33857-26-0 **MP** (°C)**:** 201
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.307E-09	1.090E-06	5	S352	2 2 0 2 2	
7.942E-09	2.010E-06	15	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
2.873E-08	7.270E-06	35	S352	2 2 0 2 2	
5.295E-08	1.340E-05	45	S352	2 2 0 2 2	

2647. $C_{12}H_6Cl_2O_2$
2,8-Dichlorodibenzo-*p*-dioxin
2,8-Dichlorodibenzodioxin
PCDD 12
3,6-Dichloro-9,10-dioxaanthracene
RN: 38964-22-6 **MP** (°C)**:** 151
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.746E-08	4.420E-06	5	S352	2 2 0 2 2	
3.394E-08	8.590E-06	15	S352	2 2 0 2 2	
6.599E-08	1.670E-05	25	S352	2 2 0 2 2	
6.614E-08	1.674E-05	25	S352	2 2 0 2 2	
1.088E-07	2.753E-05	35	S352	2 2 0 2 2	
2.035E-07	5.150E-05	45	S352	2 2 0 2 2	

2648. $C_{12}H_6Cl_2O_2$
2,3-Dichlorodibenzo-*p*-dioxin
2,3-Dichlorodibenzodioxin
PCDD 10
RN: 29446-15-9 **MP** (°C)**:** 160
MW: 253.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.454E-08	3.680E-06	5	S352	2 2 0 2 2	
2.829E-08	7.160E-06	15	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
1.201E-07	3.040E-05	35	S352	2 2 0 2 2	
2.315E-07	5.860E-05	45	S352	2 2 0 2 2	

2649. $C_{12}H_6Cl_3NO_3$
Quinonamid
2-(Dichloroacetamido)-3-chloro-1,4-naphthoquinone
HOE 13465OH
Chinonamid
2-[(Dichloroacetyl)amino]-3-chloro-1,4-naphthoquinone
RN: 27541-88-4 **MP** (°C)**:** 212.5
MW: 318.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-06	3.000E-03	23	M161	1 0 0 0 0	pH 4.6

2650. $C_{12}H_6Cl_3NO_3$
Chlornitrofen
4-Nitrophenyl 2,4,6-trichlorophenyl ether
1,3,5-Trichloro-2-(4-nitrophenoxy)benzene
1′,3′,5′-Trichlorophenyl-4-nitrophenyl ether
RN: 1836-77-7 **MP** (°C)**:**
MW: 318.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E-06	7.640E-04	22	K137	1 1 2 1 0	

2651. $C_{12}H_6Cl_4$
2,2′,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,5-tetrachloro-
PCB 48
RN: 70362-47-9 **MP** (°C)**:** 63.9
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-07	2.995E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	25	M342	1 0 1 1 2	

2652. $C_{12}H_6Cl_4$
2,3′,4,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,6-tetrachloro-
PCB 69
RN: 60233-24-1 **MP** (°C)**:** 46
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.004E-08	2.045E-05	20	M336	2 0 2 2 2	

2653. $C_{12}H_6Cl_4$
Aroclor 1254
Arochlor 1254
RN: 11097-69-1 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-07	3.900E-05	4	M336	2 0 2 2 1	
8.288E-08	2.420E-05	11.5	D085	0 0 0 0 0	
9.623E-08	2.810E-05	16.50	W033	1 0 2 2 2	
8.459E-08	2.470E-05	16.50	W033	1 0 2 2 2	
1.473E-07	4.300E-05	20	M336	2 0 2 2 1	
1.712E-07	5.000E-05	20	N326	1 0 0 0 1	
~1.92E-07	~5.60E-05	ns	H117	0 2 2 2 0	
1.541E-07	4.500E-05	ns	L106	0 0 2 1 1	
1.370E-07	4.000E-05	ns	M184	0 0 0 0 0	

2654. $C_{12}H_6Cl_4$
Aroclor 1248
Arochlor 1248
RN: 12672-29-6 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:** 357.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.425E-07	1.000E-04	20	N326	1 0 0 0 2	

2655. $C_{12}H_6Cl_4$
3,3′,5,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 3,3′,5,5′-tetrachloro-
PCB 80
RN: 33284-52-5 **MP** (°C)**:** 164
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.220E-09	1.232E-06	25	D306	2 1 2 2 2	

2656. $C_{12}H_6Cl_4$
3,3′,4,4′-Tetrachlorobiphenyl
3,4,3′,4′-Tetrachlorbiphenyl
RN: 32598-13-3 **MP** (°C)**:** 183
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-10	1.460E-07	4	D331	2 1 2 2 2	
5.000E-10	1.460E-07	4.0	M324	1 2 1 1 2	
1.490E-09	4.351E-07	20	D331	2 1 2 2 2	
1.490E-09	4.351E-07	20.0	M324	1 2 1 1 2	
6.165E-09	1.800E-06	22	O311	2 2 1 2 1	
1.404E-07	4.100E-05	23	W024	0 0 0 0 0	*sic*
1.880E-09	5.489E-07	25	D306	2 1 2 2 2	
1.950E-09	5.694E-07	25	D331	2 1 2 2 2	
1.949E-09	5.690E-07	25	D335	1 0 0 0 2	
2.569E-09	7.500E-07	25	W025	1 0 2 2 1	
1.950E-09	5.694E-07	25.0	M324	1 2 1 1 2	
4.040E-09	1.180E-06	32	D331	2 1 2 2 2	
4.040E-09	1.180E-06	32.0	M324	1 2 1 1 2	

2657. $C_{12}H_6Cl_4$
2,4,4′,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,4,4′,6-tetrachloro-
PCB 75
RN: 32598-12-2 **MP** (°C)**:** 65
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	9.110E-05	25	D306	2 1 2 2 2	

2658. $C_{12}H_6Cl_4$
2,4,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,4,4′,5-tetrachloro-
PCB 74
RN: 32690-93-0 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.049E-07	3.064E-05	20	M336	2 0 2 2 2	

2659. $C_{12}H_6Cl_4$
2,3,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4,5-tetrachloro-
PCB 61
RN: 33284-53-6 **MP** (°C)**:** 92
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.390E-08	9.900E-06	25	B319	2 0 1 2 1	
4.780E-08	1.396E-05	25	D306	2 1 2 2 2	
4.677E-08	1.366E-05	25	L322	1 1 2 2 2	
7.170E-08	2.094E-05	25	M342	1 0 1 1 2	
6.575E-08	1.920E-05	25	W025	1 0 2 2 2	
7.170E-08	2.094E-05	ns	M308	0 0 1 1 2	

2660. $C_{12}H_6Cl_4$
2,3,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4,4′-tetrachloro-
PCB 60
RN: 33025-41-1 **MP** (°C)**:** 142
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-07	3.893E-05	20	M336	2 0 2 2 2	

2661. $C_{12}H_6Cl_4$
2,3,4′,6-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4′,6-tetrachloro-
PCB 64
RN: 52663-58-8 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.207E-07	9.365E-05	20	M336	2 0 2 2 2	

2662. $C_{12}H_6Cl_4$
2,3,3′,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,3′,4′-tetrachloro-
PCB 56
RN: 41464-43-1 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-07	3.894E-05	20	M336	2 0 2 2 2	

2663. $C_{12}H_6Cl_4$
2,3′,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4,4′-tetrachloro-
PCB 66
RN: 32598-10-0 **MP** (°C)**:** 128.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.676E-05	20	M336	2 0 2 2 2	

2664. $C_{12}H_6Cl_4$
2,3′,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5-tetrachloro-
PCB 70
RN: 32598-11-1 **MP** (°C)**:** 106
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-07	3.618E-05	20	M336	2 0 2 2 2	
2.055E-07	6.000E-05	23	W024	0 0 0 0 0	
7.534E-08	2.200E-05	ns	B301	0 2 1 1 1	

2665. $C_{12}H_6Cl_4$
2,2′,6,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,6,6′-tetrachloro-
PCB 54
RN: 15968-05-5 **MP** (°C)**:** 198.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-09	2.700E-06	22	O311	2 2 1 2 1	
4.070E-08	1.188E-05	25	D306	2 1 2 2 2	

2666. $C_{12}H_6Cl_4$
2,2′,5,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,5,5′-tetrachloro-
PCB 52
RN: 35693-99-3 **MP** (°C)**:** 87
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.855E-07	1.126E-04	20	M336	2 0 2 2 2	
5.240E-08	1.530E-05	22	O311	2 2 1 2 2	
1.575E-07	4.600E-05	23	W024	0 0 0 0 0	
5.822E-07	1.700E-04	25	B319	2 0 1 2 2	
3.750E-07	1.095E-04	25	D306	2 1 2 2 2	
1.250E-07	3.650E-05	25	H341	1 0 0 0 2	
1.884E-07	5.500E-05	ns	B301	0 2 1 1 1	
9.076E-08	2.650E-05	ns	H058	0 1 2 1 2	
5.480E-08	1.600E-05	ns	M118	0 1 1 1 1	

2667. $C_{12}H_6Cl_4$
2,2′,4,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,4,4′-tetrachloro-
PCB 47
RN: 2437-79-8 **MP** (°C)**:** 42.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-07	6.600E-05	22	C413	2 0 2 2 1	
1.853E-07	5.410E-05	22	O311	2 2 1 2 2	
5.993E-07	1.750E-04	23	W024	0 0 0 0 0	
7.534E-07	2.200E-04	25	B351	1 0 0 1 1	

2668. $C_{12}H_6Cl_4$
2,3,4′,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3,4′,5-tetrachloro-
PCB 63
RN: 74472-34-7 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.997E-08	2.627E-05	20	M336	2 0 2 2 2	

2669. $C_{12}H_6Cl_4$
2,2′,5,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,5,6′-tetrachloro-
PCB 53
RN: 41464-41-9 **MP** (°C)**:** 103
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-07	1.085E-04	20	M336	2 0 2 2 2	
1.630E-07	4.759E-05	25	D306	2 1 2 2 2	

2670. $C_{12}H_6Cl_4$
2,2′,3,5′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,5′-tetrachloro-
PCB 44
RN: 41464-39-5 **MP** (°C)**:** 47
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.426E-07	1.001E-04	20	M336	2 0 2 2 2	
2.226E-07	6.500E-05	23	W024	0 0 0 0 0	
2.740E-07	8.000E-05	25	B319	2 0 1 2 0	

2671. $C_{12}H_6Cl_4$
2,2′,3,4′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4′-tetrachloro-
PCB 42
RN: 36559-22-5 **MP** (°C)**:** 68
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-07	6.083E-05	20	M336	2 0 2 2 2	

2672. $C_{12}H_6Cl_4$
2,2′,3,6′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,6′-tetrachloro-
PCB 46
RN: 41464-47-5 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E-07	1.059E-04	20	M336	2 0 2 2 2	

2673. $C_{12}H_6Cl_4$
Tetrachlorobiphenyl
1,1′-Biphenyl, tetrachloro-
Pyralene 1498
RN: 26914-33-0 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.825E-07	5.330E-05	11.5	D085	0 0 0 0 0	mixed isomers

2674. $C_{12}H_6Cl_4$
2′,3,4,5-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,3′,4′,5′-tetrachloro-
PCB 76
RN: 70362-48-0 **MP** (°C)**:** 92.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-07	5.513E-05	20	M336	2 0 2 2 2	

2675. $C_{12}H_6Cl_4$
2,2′,3,4-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,4-tetrachloro-
PCB 41
RN: 52663-59-9 **MP** (°C)**:**
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-07	6.480E-05	20	M336	2 0 2 2 2	

2676. $C_{12}H_6Cl_4$
2,2′,4,5′-Tetrachlorobiphenyl
2,2′,4′,5-Tetrachlorobiphenyl
PCB 49
RN: 41464-40-8 **MP** (°C)**:** 67
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.676E-07	7.814E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	ns	M308	0 0 1 1 2	

2677. $C_{12}H_6Cl_4$
2,2′,3,3′-Tetrachlorobiphenyl
1,1′-Biphenyl, 2,2′,3,3′-tetrachloro-
PCB 40
RN: 38444-93-8 **MP** (°C)**:** 121.0
MW: 291.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.764E-07	8.070E-05	20	M336	2 0 2 2 2	
5.822E-07	1.700E-04	23	W024	0 0 0 0 0	
5.340E-08	1.559E-05	25	D306	2 1 2 2 2	

2678. $C_{12}H_6Cl_4O_2S$
Tetradifon
2,4,5,4′-Tetrachlorodiphenyl sulfone
Tedion
Aracnol K
Akaritox
Rotetra
RN: 116-29-0 **MP** (°C)**:** 148.5
MW: 356.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.404E-07	5.000E-05	10	V301	1 0 0 0 0	
5.617E-04	2.000E-01	50	M161	1 0 0 0 0	
9.549E-07	3.400E-04	50	V301	1 0 0 0 1	

2679. $C_{12}H_7BrClNO_2$
Halacrinate
7-Bromo-5-chloro-8-quinolinyl 2-propenoate
Halocrinate
RN: 34462-96-9 **MP** (°C)**:** 100.5
MW: 312.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	6.000E-03	20	M161	1 0 0 0 0	

2680. $C_{12}H_7ClO_2$
1-Chlorodibenzo-*p*-dioxin
1-Monochlorodibenzodioxin
PCDD 1
RN: 39227-53-7 **MP** (°C)**:** 98
MW: 218.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.220E-07	1.360E-04	5	S352	2 2 0 2 2	
1.066E-06	2.330E-04	15	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
3.316E-06	7.250E-04	35	S352	2 2 0 2 2	
5.671E-06	1.240E-03	45	S352	2 2 0 2 2	

2681. $C_{12}H_7ClO_2$
2-Chlorodibenzo-*p*-dioxin
2-Monochlorodibenzo-*p*-dioxin
PCDD 2
RN: 39227-54-8 **MP** (°C)**:** 89
MW: 218.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-07	1.334E-04	3.90	D330	2 2 1 2 2	
2.904E-07	6.350E-05	5	S352	2 2 0 2 2	
6.266E-07	1.370E-04	15	S352	2 2 0 2 2	
1.363E-06	2.980E-04	25	S352	2 2 0 2 2	average of 2
1.271E-06	2.780E-04	25	S352	2 2 0 2 2	
1.460E-06	3.192E-04	25.0	D330	2 2 1 2 2	
2.987E-06	6.530E-04	35	S352	2 2 0 2 2	
3.430E-06	7.499E-04	39.0	D330	2 2 1 2 2	
5.072E-06	1.109E-03	45	S352	2 2 0 2 2	

2682. $C_{12}H_7Cl_2NO_3$
Nitrofen
2,4-Dichlorophenyl-4-nitrophenyl ether
RN: 1836-75-5 **MP** (°C)**:** 70.5
MW: 284.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.520E-06	1.000E-03	22	M061	1 0 0 0 0	
3.344E-05	9.500E-03	22	M161	1 0 0 0 0	
3.520E-06	1.000E-03	ns	B100	0 0 0 0 0	
2.144E-06	6.090E-04	ns	H322	0 0 0 0 0	

2683. $C_{12}H_7Cl_3$
2,2′,4-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,4-trichloro-
RN: 37680-66-3 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.006E-06	2.592E-04	20	M336	2 0 2 2 2	

2684. $C_{12}H_7Cl_3$
2,2′,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,6-trichloro-
RN: 38444-73-4 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-06	4.483E-04	20	M336	2 0 2 2 2	

2685. $C_{12}H_7Cl_3$
2,3′,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,3′,6-trichloro-
RN: 38444-76-7 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.498E-07	3.858E-05	20	M336	2 0 2 2 2	

2686. $C_{12}H_7Cl_3$
2,4,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,4,5-trichloro-
RN: 15862-07-4 **MP** (°C)**:** 77
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-07	8.500E-05	23	W024	0 0 0 0 0	
5.436E-07	1.400E-04	25	B319	2 0 1 2 1	
5.514E-07	1.420E-04	25	H341	1 0 0 0 2	
6.320E-07	1.628E-04	25	M342	1 0 1 1 2	
3.572E-07	9.200E-05	25	W025	1 0 2 2 1	
6.320E-07	1.628E-04	ns	M308	0 0 1 1 2	

2687. $C_{12}H_7Cl_3$
2,3,4′-Trichlorobiphenyl
1,1′-Biphenyl, 2,3,4′-trichloro-
RN: 38444-85-8 **MP** (°C)**:** 69
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-07	1.417E-04	20	M336	2 0 2 2 2	

2688. $C_{12}H_7Cl_3$
2,3,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,3,6-trichloro-
RN: 55702-45-9 **MP** (°C)**:** 49
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.126E-07	1.320E-04	20	M336	2 0 2 2 2	

2689. $C_{12}H_7Cl_3$
2,2′,3-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,3-trichloro-
RN: 38444-78-9 **MP** (°C)**:** 28.1
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-06	2.930E-04	20	M336	2 0 2 2 2	

2690. $C_{12}H_7Cl_3$
2,2′,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,2′,5-trichloro-
PCB 18
RN: 37680-65-2 **MP** (°C)**:** 44
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-06	2.986E-04	20	M336	2 0 2 2 2	
1.980E-06	5.099E-04	25	D306	2 1 2 2 2	
2.485E-06	6.400E-04	25	W025	1 0 2 2 2	
4.271E-07	1.100E-04	ns	B301	0 2 1 1 2	
9.629E-07	2.480E-04	ns	H058	0 1 2 1 2	
6.212E-08	1.600E-05	ns	M118	0 1 1 1 1	

2691. $C_{12}H_7Cl_3$
3,4,4′-Trichlorobiphenyl
3,4,4′-Trichlorbiphenyl
RN: 38444-90-5 **MP** (°C)**:** 88
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.791E-07	7.189E-05	20	M336	2 0 2 2 2	
3.106E-07	8.000E-05	23	W024	0 0 0 0 0	
5.902E-08	1.520E-05	25	W025	1 0 2 2 2	

2692. $C_{12}H_7Cl_3$
2,4′,5-Trichlorobiphenyl
2,5,4′-Trichlorobiphenyl
PCB 31
RN: 16606-02-3 **MP** (°C)**:** 67
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
3.494E-07	9.000E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	22.5	G301	0 0 0 0 0	
2.912E-07	7.500E-05	ns	B301	0 2 1 1 1	

2693. $C_{12}H_7Cl_3$
2,4,6-Trichlorobiphenyl
1,1′-Biphenyl, 2,4,6-trichloro-
RN: 35693-92-6 **MP** (°C)**:** 62.5
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	8.036E-05	4.0	D330	2 2 1 2 2	
9.800E-07	2.524E-04	25	D306	2 1 2 2 2	
9.333E-07	2.404E-04	25	L322	1 1 2 2 2	
8.760E-07	2.256E-04	25	M342	1 0 1 1 2	
7.250E-07	1.867E-04	25.0	D330	2 2 1 2 2	
1.690E-06	4.353E-04	40.0	D330	2 2 1 2 2	
8.760E-07	2.256E-04	ns	M308	0 0 1 1 2	

2694. $C_{12}H_7Cl_3$
2,4,4′-Trichlorobiphenyl
2,4,4′-PCB
RN: 7012-37-5 **MP** (°C)**:** 57
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.465E-07	1.150E-04	20	C302	1 1 2 2 2	
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
2.601E-07	6.700E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	24	C311	0 0 0 0 0	EFG
4.504E-07	1.160E-04	25	C313	0 0 0 0 0	
4.530E-07	1.167E-04	25	D306	2 1 2 2 2	
1.010E-06	2.600E-04	25	W025	1 0 2 2 2	

2695. $C_{12}H_7Cl_3$
Aroclor 1242
Arochlor 1242
RN: 53469-21-9 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.377E-07	1.900E-04	4	M336	2 0 2 2 2	
5.160E-07	1.329E-04	11.5	D085	0 0 0 0 0	
1.076E-06	2.770E-04	20	M336	2 0 2 2 2	
7.766E-07	2.000E-04	20	N326	1 0 0 0 2	
1.747E-07	4.500E-05	ns	L106	0 0 2 1 1	
7.766E-07	2.000E-04	ns	M184	0 0 0 0 0	

2696. $C_{12}H_7Cl_3$
2′,3,4-Trichlorobiphenyl
1,1′-Biphenyl, 2′,3,4-trichloro-
RN: 38444-86-9 **MP** (°C)**:** 60.0
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.147E-07	1.326E-04	20	M336	2 0 2 2 2	
1.165E-07	3.000E-05	23	W024	0 0 0 0 0	

2697. $C_{12}H_7Cl_3$
2,3′,5-Trichlorobiphenyl
1,1′-Biphenyl, 2,3′,5-trichloro-
RN: 38444-81-4 **MP** (°C)**:** 40
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E-07	1.384E-04	20	M336	2 0 2 2 2	
9.810E-07	2.527E-04	25	D306	2 1 2 2 2	

2698. $C_{12}H_7Cl_3$
Trichlorobiphenyl
Apirolio 1431C
Pyranol 1499
Pyralene 3011
RN: 25323-68-6 **MP** (°C)**:**
MW: 257.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.620E-07	1.190E-04	11.5	D085	0 0 0 0 0	mixed isomers

2699. $C_{12}H_7Cl_3O_2$
Triclosan
5-Chloro-2-(2,4-dichlorophenoxy)-phenol
RN: 3380-34-5 **MP** (°C)**:** 55.2
MW: 289.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.454E-05	1.000E-02	20	A067	1 0 0 0 0	
		amb	L434	0 0 0 0 0	
3.467E-05	1.004E-02	ns	R427	0 0 0 0 0	

2700. $C_{12}H_7NO_2$
1,8-Naphthalimide
1,8-Naphthalenedicarboximide
Naphthalimide
1,8-Naphthalenedicarboxylic acid imide
1H-Benz[de]isoquinoline-1,3(2H)-dione
RN: 81-83-4 **MP** (°C)**:** 292-300
MW: 197.20 **BP** (°C)**:** 428.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	5.916E-03	23	B410	2 1 2 2 2	

2701. $C_{12}H_7N_3O_2$
5-Nitro-1,10-phenanthroline
5-Nitro-*o*-phenanthroline
RN: 4199-88-6 **MP** (°C)**:**
MW: 225.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.210E-04	2.725E-02	25.04	B094	1 2 1 2 2	

2702. $C_{12}H_7N_5O_8$
2,4,5,6-Tetranitrodiphenylamine
RN: **MP** (°C)**:**
MW: 349.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-04	8.199E-02	13.5	D070	1 2 0 0 1	
2.949E-04	1.030E-01	50	D070	1 2 0 0 2	
5.783E-04	2.020E-01	100	D070	1 2 0 0 2	

2703. $C_{12}H_7N_5O_8$
2,4,2′,4′-Tetranitrodiphenylamine
2,4,2′,4-Tetranitro-diphenylamin
RN: 2908-76-1 **MP** (°C)**:**
MW: 349.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.727E-04	2.000E-01	100	F300	1 0 0 0 2	

2704. $C_{12}H_8$
Acenaphthylene
1,2-Dehydroacenaphthalene
Acenaphthalene
RN: 208-96-8 **MP** (°C)**:** 93.5–94.5
MW: 152.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-05	3.930E-03	25	L332	1 1 1 1 2	

2705. $C_{12}H_8Br_2$
4,4′-Dibromobiphenyl
p,p′-Dibromobiphenyl
RN: 92-86-4 **MP** (°C)**:** 170
MW: 312.02 **BP** (°C)**:** 357

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-02	5.743E+00	26.5	G312	0 0 0 0 0	

2706. $C_{12}H_8Br_2O$
4,4′-Dibromodiphenylether
bis-p-Bromophenyl ether
Dibromodiphenyl ether, *p,p′*-
RN: 2050-47-7 **MP** (°C)**:** 59 C
MW: 328.01 **BP** (°C)**:** 357 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.878E-07	9.440E-05	10	K431	0 0 0 0 0	
6.585E-07	2.160E-04	25	K431	0 0 0 0 0	
1.171E-06	3.840E-04	35	K431	0 0 0 0 0	

2707. $C_{12}H_8Cl_2$
2,5-Dichlorobiphenyl
1,1′-Biphenyl, 2,5-dichloro-
RN: 34883-39-1 **MP** (°C)**:** 23
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.454E-06	1.440E-03	23	W024	0 0 0 0 0	
5.000E-06	1.116E-03	25	D306	2 1 2 2 2	
8.700E-06	1.941E-03	25	M342	1 0 1 1 1	
2.600E-06	5.800E-04	25	W025	1 0 2 2 2	
8.516E-07	1.900E-04	ns	B301	0 2 1 1 2	
2.680E-05	5.979E-03	ns	M308	0 0 1 1 2	

2708. $C_{12}H_8Cl_2$
2,4-Dichlorobiphenyl
1,1′-Biphenyl, 2,4-dichloro-
RN: 33284-50-3 **MP** (°C)**:** 25.0
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.747E-06	6.129E-04	20	M336	2 0 2 2 2	
3.138E-07	7.000E-05	23	W024	0 0 0 0 0	*sic*
5.065E-06	1.130E-03	25	B319	2 0 1 2 2	
5.065E-06	1.130E-03	25	B350	1 0 0 0 2	
5.150E-06	1.149E-03	25	D306	2 1 2 2 2	

2709. $C_{12}H_8Cl_2$
2,4′-Dichlorobiphenyl
2,4′-PCB
RN: 34883-43-7 **MP** (°C)**:** 43
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-06	6.370E-04	20	C302	1 1 2 2 2	
2.413E-06	5.383E-04	20	M336	2 0 2 2 2	
2.241E-06	5.000E-04	24	H100	2 0 2 2 0	
2.779E-06	6.200E-04	25	W025	1 0 2 2 2	
2.855E-06	6.370E-04	ns	H058	0 1 2 1 2	

2710. $C_{12}H_8Cl_2$
2,3′-Dichlorobiphenyl
1,1′-Biphenyl, 2,3′-dichloro-
RN: 25569-80-6 **MP** (°C)**:**
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-06	5.798E-04	20	M336	2 0 2 2 2	

2711. $C_{12}H_8Cl_2$
2,6-Dichlorobiphenyl
1,1′-Biphenyl, 2,6-dichloro-
PCB 10
RN: 33146-45-1 **MP** (°C)**:** 35
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-06	5.400E-04	22	O311	2 2 1 2 2	
1.080E-05	2.410E-03	25	D306	2 1 2 2 2	
6.230E-06	1.390E-03	25	M342	1 0 1 1 2	
6.230E-06	1.390E-03	ns	M308	0 0 1 1 2	

2712. $C_{12}H_8Cl_2$
2,2′-Dichlorobiphenyl
2,2′-PCB
RN: 13029-08-8 **MP** (°C)**:** 61
MW: 223.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.214E-06	7.170E-04	20	C302	1 1 2 2 2	
5.038E-06	1.124E-03	20	M336	2 0 2 2 2	
3.541E-06	7.900E-04	22.5	G301	0 0 0 0 0	

(*continued*)

2712. $C_{12}H_8Cl_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.275E-06	1.400E-03	23	W024	0 0 0 0 0	
4.034E-06	9.000E-04	24	H100	2 0 2 2 0	
5.410E-06	1.207E-03	25	D306	2 1 2 2 2	
3.541E-06	7.900E-04	25	W025	1 0 2 2 2	

2713. $C_{12}H_8Cl_2$

3,4-Dichlorobiphenyl
1,1′-Biphenyl, 3,4-dichloro-
RN: 2974-92-7 **MP** (°C)**:** 49.5
MW: 223.10 **BP** (°C)**:** 197.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.550E-08	7.920E-06	25	D306	2 1 2 2 2	
4.074E-07	9.089E-05	ns	R424	0 0 0 0 0	

2714. $C_{12}H_8Cl_2$

4,4′-Dichlorobiphenyl
4,4′-PCB
Dichlorobiphenyl
RN: 2050-68-2 **MP** (°C)**:** 149
MW: 223.10 **BP** (°C)**:** 317

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.488E-06	3.320E-04	11.5	D085	0 0 0 0 0	mixed isomers
2.779E-07	6.200E-05	20	C053	0 0 0 0 0	
2.779E-07	6.200E-05	20	F071	1 1 1 1 1	
2.779E-07	6.200E-05	20	M344	1 0 0 0 1	
2.689E-07	6.000E-05	24	H100	2 0 2 2 0	
2.376E-07	5.300E-05	25	B319	2 0 1 2 2	average of 2
2.062E-07	4.600E-05	25	B350	1 0 0 0 1	
1.630E-07	3.637E-05	25	D306	2 1 2 2 2	
2.913E-07	6.500E-05	25	H341	1 0 0 0 1	
2.510E-07	5.600E-05	25	W025	1 0 2 2 1	

2715. $C_{12}H_8Cl_2$

3,3′-Dichlorobiphenyl
1,1′-Biphenyl, 3,3′-dichloro-
RN: 2050-67-1 **MP** (°C)**:** 29
MW: 223.10 **BP** (°C)**:** 323.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-06	3.547E-04	25	D306	2 1 2 2 2	

2716. $C_{12}H_8Cl_2O_2S$

bis(4-Chlorophenyl) sulfone
4,4′-Dichlorodiphenyl sulfone
1,1′-Sulfonylbis(4-chlorobenzene)
p-Chlorophenyl sulfone

RN: 80-07-9 **MP** (°C)**:** 149 C
MW: 287.17 **BP** (°C)**:** 397 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-07	5.000E-05	22	J420	0 0 0 0 0	pH 6.5

2717. $C_{12}H_8Cl_6$

Aldrin
1,2,3,4,10,10-Hexachloro-1,4,4α,5,8,8α-hexahydro-1,4:5,8-dimethanonaphthalene
Aldrite
Seedrin
Aldrosol
HHDN

RN: 309-00-2 **MP** (°C)**:** 104.3
MW: 364.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.877E-07	1.050E-04	15	B083	2 2 1 2 2	particle size 5 µm
7.413E-08	2.705E-05	20	B179	0 0 0 0 0	
4.659E-08	1.700E-05	22.5	G301	0 0 0 0 0	
4.898E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.933E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 µm
5.481E-07	2.000E-04	25	M130	1 0 0 0 0	
4.659E-08	1.700E-05	25	W025	1 0 2 2 2	
7.399E-08	2.700E-05	26.5	P027	1 1 2 2 1	
5.481E-07	2.000E-04	26.70	L095	2 2 1 1 2	
7.399E-08	2.700E-05	27	M161	0 0 0 0 1	
9.591E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.644E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 µm
7.399E-08	2.700E-05	ns	I308	0 0 0 0 0	
3.562E-08	1.300E-05	ns	K138	0 0 0 0 2	
1.096E-07	4.000E-05	ns	M110	0 0 0 0 0	EFG

2718. $C_{12}H_8Cl_6O$

Endrin
1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4α,5,6,7,8,8α-octahydro-1,4-*endo*-*endo*-5,8-dimethanonaphthalene
Mendrin
Nendrin

RN: 72-20-8 **MP** (°C)**:** 228.0
MW: 380.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.413E-07	1.300E-04	15	B083	2 2 1 2 2	particle size 5 µm
6.607E-07	2.517E-04	24.99	K436	0 0 0 0 0	
6.563E-07	2.500E-04	25	B083	2 2 1 2 2	particle size 5 µm
6.826E-07	2.600E-04	25	W025	1 0 2 2 2	
1.103E-06	4.200E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.641E-06	6.250E-04	45	B083	2 2 1 2 2	particle size 5 µm
6.301E-08	2.400E-05	ns	K138	0 0 0 0 2	
1.050E-06	4.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
6.563E-07	2.500E-04	ns	V414	0 0 0 0 0	

2719. $C_{12}H_8Cl_6O$

Dieldrin
3,4,5,6,9,9-Hexachloro-1α,2,2α,3,6,6α,7,7α-octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene
Alvit
Quintox
Oxralox

RN: 60-57-1 **MP** (°C)**:** 175.5
MW: 380.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-07	7.999E-05	10	B324	0 0 0 0 0	
2.100E-07	8.000E-05	10	B324	0 0 0 0 0	
2.363E-07	9.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
4.898E-07	1.866E-04	20	B179	0 0 0 0 0	
3.675E-07	1.400E-04	20	B324	0 0 0 0 0	
3.676E-07	1.400E-04	20	B324	0 0 0 0 0	
1.229E-06	4.680E-04	22	K137	1 1 2 1 0	
5.129E-07	1.954E-04	24.99	K436	0 0 0 0 0	
5.119E-07	1.950E-04	25	B083	2 2 1 2 2	particle size 5 µm
4.883E-07	1.860E-04	25	I308	0 0 0 0 0	
6.563E-07	2.500E-04	25	M130	1 0 0 0 1	
5.251E-07	2.000E-04	25	W025	1 0 2 2 2	
1.313E-07	5.000E-05	26	M061	1 0 0 0 0	
4.883E-07	1.860E-04	26.5	P027	1 1 2 2 2	
5.251E-07	2.000E-04	27	B161	2 1 2 2 0	EFG
4.883E-07	1.860E-04	27	M161	0 0 0 0 2	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	

(*continued*)

2719. $C_{12}H_8Cl_6O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-06	4.000E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.313E-06	5.000E-04	40	B161	2 1 2 2 0	EFG
1.706E-06	6.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
2.363E-06	9.000E-04	50	B161	2 1 2 2 0	EFG
3.544E-06	1.350E-03	60	B161	2 1 2 2 0	EFG
6.511E-06	2.480E-03	70	B161	2 1 2 2 0	EFG
6.563E-07	2.500E-04	ns	H322	0 0 0 0 0	
5.776E-08	2.200E-05	ns	K138	0 0 0 0 2	
7.876E-07	3.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
5.119E-07	1.950E-04	ns	V414	0 0 0 0 0	

2720. $C_{12}H_8N_2$

p-Phenanthroline
p-Phenanthrolin
RN: 230-07-9 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.442E+00	ns	K114	0 0 0 0 0	

2721. $C_{12}H_8N_2$

Phenazine
Dibenzopyrazine
RN: 92-82-0 **MP** (°C)**:** 175.5
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	2.523E-02	25	K009	1 2 1 1 0	EFG

2722. $C_{12}H_8N_2$

o-Phenanthroline
1,10-Phenanthroline
o-Phenanthrolin
RN: 66-71-7 **MP** (°C)**:** 115
MW: 180.21 **BP** (°C)**:** >300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-02	3.340E+00	24.99	B444	0 0 0 0 0	
1.526E-02	2.750E+00	25	M155	1 0 1 1 0	EFG
1.490E-02	2.685E+00	25.04	B094	1 2 1 2 2	
1.850E-02	3.334E+00	31	B094	1 2 1 2 2	

(*continued*)

2722. $C_{12}H_8N_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-02	3.766E+00	35	B094	1 2 1 2 2	
2.550E-02	4.595E+00	40.04	B094	1 2 1 2 2	
2.880E-02	5.190E+00	45.44	B094	1 2 1 2 2	
3.410E-02	6.145E+00	50.04	B094	1 2 1 2 2	

2723. $C_{12}H_8N_2$
m-Phenanthroline
m-Phenanthrolin
RN: 230-46-6 **MP** (°C)**:**
MW: 180.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	7.208E-01	ns	K114	0 0 0 0 0	

2724. $C_{12}H_8N_4O_2$
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-benzoyl-1,5-dihydro-
RN: 96448-63-4 **MP** (°C)**:**
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.828E-05	1.400E-02	22	B428	1 2 1 2 1	

2725. $C_{12}H_8N_4O_6$
Picrylaniline
2,4,6-Trinitrodiphenyllamine
RN: 2919-12-2 **MP** (°C)**:**
MW: 304.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-05	1.791E-02	25	B335	1 2 0 0 1	

2726. $C_{12}H_8O$
Dibenzofuran
Diphenylene oxide
DBF
RN: 132-64-9 **MP** (°C)**:** 83
MW: 168.20 **BP** (°C)**:** 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.820E-06	1.652E-03	4.0	D330	2 2 1 2 2	
5.960E-05	1.002E-02	25	B173	2 0 2 2 2	

(*continued*)

2726. $C_{12}H_8O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.112E-03	25	L301	1 1 2 2 2	
2.592E-05	4.360E-03	25	O406	0 0 0 0 0	
2.812E-05	4.730E-03	25	O406	0 0 0 0 0	
2.510E-05	4.222E-03	25.0	D330	2 2 1 2 2	
4.140E-05	6.963E-03	39.8	D330	2 2 1 2 2	

2727. $C_{12}H_8O_2$

Dibenzo-*p*-dioxin
Dibenzo[1,4]dioxin
Oxanthrene
Phenodioxin

RN: 262-12-4 **MP** (°C)**:** 119
MW: 184.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-06	2.118E-04	4.10	D330	2 2 1 2 2	
1.113E-06	2.050E-04	5	S352	2 2 0 2 2	
2.497E-06	4.600E-04	15	S352	2 2 0 2 2	
7.601E-06	1.400E-03	25	O406	0 0 0 0 0	
6.841E-06	1.260E-03	25	O406	0 0 0 0 0	
4.729E-06	8.710E-04	25	S352	2 2 0 2 2	average of 2
4.571E-06	8.420E-04	25	S352	2 2 0 2 2	
4.890E-06	9.007E-04	25.0	D330	2 2 1 2 2	
9.566E-06	1.762E-03	35	S352	2 2 0 2 2	
1.300E-05	2.395E-03	40.0	D330	2 2 1 2 2	
1.771E-05	3.262E-03	45	S352	2 2 0 2 2	

2728. $C_{12}H_8O_4$

Methoxsalen
Ammoidin
8-Methoxy-2′,3′,6,7-furocoumarin
Methoxalen
8-Methoxyfuranocoumarin
Oxypsoralen

RN: 298-81-7 **MP** (°C)**:** 148
MW: 216.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	4.756E-02	30	E012	1 2 1 1 0	

2729. $C_{12}H_8S$

Dibenzothiophene
Diphenylene sulfide

RN: 132-65-0 **MP** (°C)**:** 97
MW: 184.26 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.978E-06	1.470E-03	24	H106	1 0 2 2 2	
7.978E-06	1.470E-03	24	M303	1 0 1 1 2	
2.871E-06	5.291E-04	25	L301	1 1 2 2 2	
7.978E-06	1.470E-03	ns	H107	0 0 0 0 2	

2730. $C_{12}H_9Br$

4-Bromobiphenyl
1,1′-Biphenyl, 4-bromo-
Bromodiphenyl

RN: 92-66-0 **MP** (°C)**:** 91.5
MW: 233.11 **BP** (°C)**:** 310.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-06	2.354E-04	4.0	D330	2 2 1 2 2	
2.800E-06	6.527E-04	25.0	D330	2 2 1 2 2	
3.740E-06	8.718E-04	40.0	D330	2 2 1 2 2	

2731. $C_{12}H_9Cl$

2-Chlorobiphenyl
2-PCB

RN: 2051-60-7 **MP** (°C)**:** 32
MW: 188.66 **BP** (°C)**:** 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-05	3.760E-03	20	C302	1 1 2 2 2	
3.074E-05	5.800E-03	23	W024	0 0 0 0 0	
4.771E-06	9.000E-04	24	H100	2 0 2 2 0	
4.134E-05	7.800E-03	25	B351	1 0 0 1 1	
2.680E-05	5.056E-03	25	M342	1 0 1 1 2	
2.189E-05	4.130E-03	25	W025	1 0 2 2 2	
2.680E-05	5.056E-03	ns	M308	0 0 1 1 2	

2732. $C_{12}H_9Cl$
4-Chlorobiphenyl
1-Chloro-4-phenyl benzene
4-Monochloro-biphenyl
RN: 2051-62-9 **MP** (°C)**:** 77
MW: 188.66 **BP** (°C)**:** 291

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.202E-06	1.170E-03	23	W024	0 0 0 0 0	
2.120E-06	4.000E-04	24	H100	2 0 2 2 0	
7.103E-06	1.340E-03	25	B319	2 0 1 2 2	average of 2
6.891E-06	1.300E-03	25	B350	1 0 0 0 2	
6.361E-06	1.200E-03	25	B351	1 0 0 1 1	
6.361E-06	1.200E-03	25	H341	1 0 0 0 2	
7.087E-06	1.337E-03	25	L322	1 1 2 2 2	average of 2
7.079E-06	1.336E-03	25	L322	1 1 2 2 2	average of 2
4.771E-06	9.000E-04	25	W025	1 0 2 2 2	

2733. $C_{12}H_9Cl$
3-Chlorobiphenyl
3-Chlorbiphenyl
RN: 2051-61-8 **MP** (°C)**:** 16
MW: 188.66 **BP** (°C)**:** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.908E-05	3.600E-03	23	W024	0 0 0 0 0	
9.806E-06	1.850E-03	23	W024	0 0 0 0 0	
1.924E-05	3.630E-03	25	B319	2 0 1 2 2	
6.891E-06	1.300E-03	25	W025	1 0 2 2 2	

2734. $C_{12}H_9Cl$
Aroclor 1221
Arochlor 1221
RN: 11104-28-2 **MP** (°C)**:**
MW: 188.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.06E-06	>2.00E-04	ns	M184	0 0 0 0 0	

2735. $C_{12}H_9ClF_3N_3O$

Norflurazon
4-Chloro-5-(methylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3(2H)-pyridazinone
Zorial
RN: 27314-13-2 **MP** (°C)**:** 177
MW: 303.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.220E-05	2.800E-02	23	M161	1 0 0 0 1	
9.220E-05	2.800E-02	24	C105	2 1 2 2 2	
9.220E-05	2.800E-02	25	B310	1 1 0 0 1	

2736. $C_{12}H_9ClN_2$

4-Chloroazobenzene
Diazene, (4-chlorophenyl)phenyl-, (E)-
RN: 4340-77-6 **MP** (°C)**:** 88
MW: 216.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	4.333E-04	25	B333	0 0 0 0 0	

2737. $C_{12}H_9ClO$

4-Chlorophenyl phenyl ether
1-Chloro-4-phenoxybenzene
p-Chlorodiphenyl oxide
RN: 7005-72-3 **MP** (°C)**:**
MW: 204.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.612E-05	3.300E-03	25	B131	1 0 0 0 1	

2738. $C_{12}H_9Cl_2NO_2S$

N-(2,3-Chlorophenyl)-benzene-sulfonamide
RN: **MP** (°C)**:**
MW: 302.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-05	5.809E-03	20	P433	0 0 0 0 0	
2.256E-05	6.816E-03	25	P433	0 0 0 0 0	
2.717E-05	8.209E-03	30	P433	0 0 0 0 0	
3.511E-05	1.061E-02	37	P433	0 0 0 0 0	
4.300E-05	1.299E-02	42	P433	0 0 0 0 0	

2739. $C_{12}H_9Cl_2NO_3$
Vinclozolin
3-(3,5-Dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione
Ornalin
Vinclozalin
Ronilan
RN: 50471-44-8 **MP** (°C)**:** 108
MW: 286.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.495E-03	1.000E+00	20	M161	1 0 0 0 0	
9.120E-06	2.609E-03	ns	R427	0 0 0 0 0	

2740. $C_{12}H_9Cl_3NO_2S$
Reserptyl
4′-[Chlorophenyl}-3,4-dichlorophenylbenzene-sulphonamide
RN: **MP** (°C)**:** 127–129
MW: 337.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-04	3.600E-02	25	L014	1 0 1 1 1	

2741. $C_{12}H_9FN_2O_4$
1-Benzyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, phenylmethyl ester
RN: 66999-98-2 **MP** (°C)**:**
MW: 264.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-04	8.000E-02	22	B332	1 1 0 0 1	pH 4.0

2742. $C_{12}H_9N$
Carbazole
9-Azafluorene
Dibenzo[b,d]pyrrole
Diphenylenimine
9H-Carbazole
Dibenzopyrrole
RN: 86-74-8 **MP** (°C)**:** 245
MW: 167.21 **BP** (°C)**:** 355

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.177E-06	1.200E-03	20	H300	1 1 2 2 1	
5.427E-06	9.075E-04	25	L301	1 1 2 2 2	

2743. $C_{12}H_9NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-methyl-
RN: 74103-11-0 **MP** (°C)**:**
MW: 215.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-07	7.000E-05	25	P089	0 0 0 0 0	
4.321E-07	9.300E-05	37	P089	0 0 0 0 0	
5.529E-07	1.190E-04	51	P089	0 0 0 0 0	

2744. $C_{12}H_9NS$
Phenothiazine
Dibenzo-1,4-thiazine
Thiodiphenylamine
RN: 92-84-2 **MP** (°C)**:** 185.1
MW: 199.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.196E-03	20	M177	2 2 2 2 0	EFG
8.000E-06	1.594E-03	25	M177	2 2 2 2 0	EFG
1.000E-05	1.993E-03	30	M177	2 2 2 2 0	EFG

2745. $C_{12}H_9N_3O_2$
4-Nitroazobenzene
Diazene, (*p*-nitrophenyl)phenyl-, (E)-
RN: 2491-52-3 **MP** (°C)**:**
MW: 227.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	6.362E-04	25	B333	0 0 0 0 0	

2746. $C_{12}H_9N_3O_3$
Dis. A. 3
4-[(4-Nitrophenyl)azo]phenol
p-Nitrophenylazophenol
p-Hydroxy-*p′*-nitroazobenzene
RN: 1435-60-5 **MP** (°C)**:** 216
MW: 243.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.892E-03	25	B333	0 0 0 0 0	

2747. $C_{12}H_9N_3O_4$
2,4-Dinitrodiphenylamine
2,4-Dinitrodiphenylamin
C.I. Disperse yellow 14
RN: 961-68-2 **MP** (°C)**:** 160
MW: 259.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.466E-04	3.800E-02	15	D070	1 2 0 0 1	
1.543E-04	4.000E-02	15	F300	1 0 0 0 0	
5.100E-06	1.322E-03	25	B333	0 0 0 0 0	*sic*
3.240E-04	8.399E-02	50	D070	1 2 0 0 1	
5.516E-04	1.430E-01	100	D070	1 2 0 0 2	

2748. $C_{12}H_9N_3O_5$
C.I. Disperse yellow 1
C.I. Disperse yellow 1
p-(2,4-Dinitroanilino)
2,4-Dinitro-4′-hydroxydiphenylamine
4-Hydroxy-2′,4′-dinitrodiphenylamine
RN: 119-15-3 **MP** (°C)**:** 194
MW: 275.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-06	2.477E-03	25	B333	0 0 0 0 0	
6.195E-05	1.705E-02	60	P313	0 0 0 0 0	average of 2
1.546E-04	4.255E-02	70	P313	0 0 0 0 0	average of 2
2.954E-04	8.130E-02	80	P313	0 0 0 0 0	average of 2
5.559E-04	1.530E-01	90	P313	0 0 0 0 0	average of 2
1.163E-03	3.200E-01	100	P313	0 0 0 0 0	

2749. $C_{12}H_9N_5O_3$
1-Nicotinoyloxymethyl allopurinol
3-Pyridinecarboxylic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester
RN: 98846-66-3 **MP** (°C)**:** 242–243
MW: 271.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.429E-04	9.300E-02	22	B322	0 0 0 0 0	

2750. $C_{12}H_{10}$

Diphenyl
Biphenyl
Phenylbenzene
1,1′-Biphenyl
Lemonene

RN: 92-52-4 **MP** (°C)**:** 69.1
MW: 154.21 **BP** (°C)**:** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E-05	2.650E-03	–.7	N053	1 0 0 1 0	EFG
1.973E-05	3.042E-03	4.62	N053	1 0 0 1 0	EFG
2.670E-05	4.118E-03	10	J302	2 1 2 2 2	
2.372E-05	3.658E-03	10.13	N053	1 0 0 1 0	EFG
2.918E-05	4.500E-03	14.20	N053	1 0 0 1 0	EFG
3.800E-05	5.860E-03	20	H306	1 0 1 2 1	
4.182E-05	6.450E-03	20	T301	1 2 2 2 2	
3.590E-05	5.536E-03	20.10	N053	1 0 0 1 0	EFG
4.100E-05	6.323E-03	21	A057	2 1 2 2 1	
4.533E-05	6.990E-03	22	C413	2 0 2 2 1	
4.850E-05	7.480E-03	22.5	G301	0 0 0 0 0	
1.187E-04	1.830E-02	23.5	S171	2 1 2 2 2	
2.983E-05	4.600E-03	24	H100	2 0 2 2 1	
5.512E-05	8.500E-03	24	H116	2 1 0 0 2	
4.708E-05	7.260E-03	24.60	W003	2 2 2 2 2	average of 3
3.852E-05	5.940E-03	25	A001	1 0 2 2 2	
4.570E-05	7.048E-03	25	A325	2 1 2 2 2	
4.850E-05	7.480E-03	25	B003	2 2 2 2 2	
3.910E-05	6.030E-03	25	B173	2 0 2 2 2	
4.799E-05	7.400E-03	25	B319	2 0 1 2 1	average of 2
4.409E-05	6.800E-03	25	B351	1 0 0 1 1	
4.831E-05	7.450E-03	25	E004	2 1 2 2 2	
4.850E-05	7.479E-03	25	J302	2 1 2 2 2	
4.863E-05	7.500E-03	25	M040	1 0 0 1 1	
4.539E-05	7.000E-03	25	M064	1 1 2 2 1	
4.850E-05	7.480E-03	25	M130	1 0 0 0 2	
4.350E-05	6.708E-03	25	M342	1 0 1 1 2	
4.540E-05	7.001E-03	25	M342	1 0 1 1 2	
4.234E-04	6.530E-02	25	S005	2 2 2 2 2	
4.910E-05	7.572E-03	25.04	V013	2 2 2 2 2	
4.416E-05	6.811E-03	25.35	N053	1 0 0 1 0	EFG
5.689E-05	8.774E-03	28.95	N053	1 0 0 1 0	EFG
5.700E-05	8.790E-03	29.90	W003	2 2 2 2 2	average of 3
5.525E-05	8.520E-03	30.30	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	38.40	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	40.10	W003	2 2 2 2 2	average of 3
1.219E-04	1.880E-02	47.50	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.10	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.20	W003	2 2 2 2 2	average of 2
1.855E-04	2.860E-02	54.70	W003	2 2 2 2 2	average of 3

(*continued*)

2750. $C_{12}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-04	3.620E-02	59.20	W003	2 2 2 2 2	average of 3
2.620E-04	4.040E-02	60.50	W003	2 2 2 2 2	
2.918E-04	4.500E-02	64.50	W003	2 2 2 2 2	average of 3
4.539E-05	7.000E-03	ns	H123	0 0 0 0 0	
4.350E-05	6.708E-03	ns	M308	0 0 1 1 2	
4.539E-05	7.000E-03	ns	M344	0 0 0 0 1	

2751. $C_{12}H_{10}$

Acenaphthene
1,2-Dihydroacenaphthene
1,8-Ethylenenaphthalene
peri-Ethylenenaphthalene

RN: 83-32-9 **MP** (°C)**:** 95
MW: 154.21 **BP** (°C)**:** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.315E-05	3.570E-03	22.20	W003	2 2 2 2 2	
4.780E-05	7.371E-03	25	B173	2 0 2 2 2	
2.250E-05	3.470E-03	25	E004	2 1 2 2 2	
2.218E-05	3.420E-03	25	L332	1 1 1 1 2	
2.548E-05	3.930E-03	25	M064	1 1 2 2 2	
2.550E-05	3.932E-03	25	M342	1 0 1 1 2	
8.889E-07	1.371E-04	25	R084	2 2 2 2 1	*sic*
2.330E-05	3.593E-03	25.04	V013	2 2 2 2 2	
3.041E-05	4.690E-03	30.00	W003	2 2 2 2 2	average of 3
3.761E-05	5.800E-03	34.50	W003	2 2 2 2 2	average of 3
4.520E-05	6.970E-03	39.30	W003	2 2 2 2 1	average of 3
6.076E-05	9.370E-03	44.70	W003	2 2 2 2 1	average of 3
8.060E-05	1.243E-02	50.10	W003	2 2 2 2 2	average of 3
1.038E-04	1.600E-02	55.60	W003	2 2 2 2 2	average of 3
1.741E-04	2.685E-02	64.50	W003	2 2 2 2 2	average of 3
1.511E-04	2.330E-02	65.20	W003	2 2 2 2 2	average of 3
2.118E-04	3.267E-02	69.80	W003	2 2 2 2 2	average of 3
2.283E-04	3.520E-02	71.90	W003	2 2 2 2 2	
2.568E-04	3.960E-02	73.40	W003	2 2 2 2 2	average of 2
2.597E-04	4.005E-02	74.70	W003	2 2 2 2 2	average of 2
3.981E-05	6.139E-03	ns	D001	0 0 0 0 2	
2.248E-05	3.467E-03	ns	I332	0 0 0 0 1	
2.000E-05	3.084E-03	ns	L060	0 0 0 0 0	average
2.548E-05	3.930E-03	ns	M344	0 0 0 0 2	
2.344E-05	3.615E-03	ns	R424	0 0 0 0 0	

2752. $C_{12}H_{10}ClN$

4-Amino-4′-chlorodiphenyl
4-Chloro-4′-aminobiphenyl
p-Amino-*p*′-chlorobiphenyl
p′-Chloro-*p*-phenylaniline

RN: 135-68-2 **MP** (°C)**:**
MW: 203.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	4.684E-03	ns	B305	0 2 0 0 1	

2753. $C_{12}H_{10}ClNO_2S$

N-(2-Chlorophenyl)-benzene-sulfonamide

RN: **MP** (°C)**:**
MW: 267.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-05	1.119E-02	20	P433	0 0 0 0 0	
4.800E-05	1.285E-02	25	P433	0 0 0 0 0	
5.239E-05	1.403E-02	30	P433	0 0 0 0 0	
5.667E-05	1.517E-02	37	P433	0 0 0 0 0	
6.444E-05	1.725E-02	42	P433	0 0 0 0 0	

2754. $C_{12}H_{10}ClNO_2S$

N-(4-Chlorophenyl)-benzene-sulfonamide

RN: **MP** (°C)**:**
MW: 267.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.611E-05	2.038E-02	20	P433	0 0 0 0 0	
9.333E-05	2.499E-02	25	P433	0 0 0 0 0	
1.244E-04	3.332E-02	30	P433	0 0 0 0 0	
1.789E-04	4.789E-02	37	P433	0 0 0 0 0	
2.189E-04	5.860E-02	42	P433	0 0 0 0 0	

2755. $C_{12}H_{10}Cl_2N_2$

3,3′-Dichlorobenzidine
3,3′-Dichloro-4,4′-biphenyldiamine
o,*o*′-Dichlorobenzidine
4,4′-Diamino-3,3′-dichlorobiphenyl

RN: 91-94-1 **MP** (°C)**:** 132
MW: 253.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.114E-03	25	B173	2 0 2 2 2	
<3.95E-06	<1.00E-03	30	M311	1 1 2 2 0	

2756. $C_{12}H_{10}N_2$
Harmane
1-Methyl-9H-pyrido[3,4-b]indole
Aribine
RN: 486-84-0 **MP** (°C)**:** 235–238
MW: 182.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.010E+00	1.095E+03	15	B413	1 0 2 2 1	
6.250E+00	1.139E+03	16	B413	1 0 2 2 1	
6.710E+00	1.223E+03	17	B413	1 0 2 2 1	
8.360E+00	1.523E+03	20	B413	1 0 2 2 1	
1.364E+01	2.486E+03	37	B413	1 0 2 2 1	
1.434E+01	2.613E+03	38	B413	1 0 2 2 1	
1.617E+01	2.947E+03	45	B413	1 0 2 2 1	

2757. $C_{12}H_{10}N_2O$
4-Phenylazophenol
4-Hydroxyazobenzene
p-Hydroxyazobenzene
C.I. Solvent yellow 7
RN: 1689-82-3 **MP** (°C)**:** 150
MW: 198.23 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.540E-04	9.000E-02	20	F300	1 0 0 0 1	
1.100E-04	2.180E-02	25	B333	0 0 0 0 0	
1.715E-04	3.400E-02	37	H120	1 1 1 1 1	normal saline
4.036E-03	8.000E-01	100	F300	1 0 0 0 1	

2758. $C_{12}H_{10}N_2O$
Diphenylnitrosamine
Redax
N-Nitroso-*N*-phenylaniline
RN: 86-30-6 **MP** (°C)**:** 67
MW: 198.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-04	3.509E-02	25	B173	2 0 2 2 2	

2759. $C_{12}H_{10}N_2O_2$
2,4-Dihydroxyazobenzene
2,4-Dihydroxy-azobenzol
RN: 2051-85-6 **MP** (°C)**:** 170
MW: 214.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.336E-04	2.000E-01	20	F300	1 0 0 0 0	

2760. $C_{12}H_{10}N_2O_3$
3-Hydroxyazobenzene
3-Hydroxy-azobenzol
RN: 40038-46-8 **MP** (°C)**:**
MW: 230.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.475E-03	8.000E-01	100	F300	1 0 0 0 1	

2761. $C_{12}H_{10}N_4O_2$
C.I. Disperse orange 3
4′-Nitro-4-aminoazobenzene
4-Amino-4′-nitroazobenzene
4-(4-Nitrophenylazo)aniline
RN: 730-40-5 **MP** (°C)**:** 211
MW: 242.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.907E-04	25	B333	0 0 0 0 0	

2762. $C_{12}H_{10}N_4O_4$
C.I. Disperse yellow 9
2,4-Dinitro-4′-aminodiphenylamine
4-Amino-2′,4′-dinitrodiphenylamine
C.I. 10375
RN: 6373-73-5 **MP** (°C)**:** 188
MW: 274.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.645E-03	25	B333	0 0 0 0 0	

2763. $C_{12}H_{10}O$
p-Phenylphenol
p-Hydroxybiphenyl
RN: 92-69-3 **MP** (°C)**:** 164.5
MW: 170.21 **BP** (°C)**:** 306.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	5.617E-02	25	E014	2 2 2 1 2	pH 7.2
5.875E-05	1.000E-02	25	L021	1 0 0 0 0	

2764. $C_{12}H_{10}O$
o-Phenylphenol
2-Phenylphenol
RN: 90-43-7 **MP** (°C)**:** 56.5
MW: 170.21 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.790E-04	1.666E-01	25	L021	1 0 0 0 0	
4.110E-03	6.995E-01	25	M061	0 0 0 0 0	
4.112E-03	7.000E-01	25	M161	1 0 0 0 0	
3.162E-04	5.383E-02	rt	D056	0 1 1 1 0	EFG, pH 6–8, *sic*

2765. $C_{12}H_{10}O$
Phenyl ether
Diphenyl ether
RN: 101-84-8 **MP** (°C)**:** 28
MW: 170.21 **BP** (°C)**:** 259

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.341E-02	3.984E+00	25	B019	1 0 1 2 0	*sic*
1.060E-04	1.804E-02	25	B173	2 0 2 2 2	
1.234E-04	2.100E-02	25	F071	1 1 2 1 1	
1.100E-04	1.872E-02	25.04	V013	2 2 2 2 2	

2766. $C_{12}H_{10}O_2$
1-Naphthaleneacetic acid
NAA
RN: 86-87-3 **MP** (°C)**:** 134
MW: 186.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.040E-03	3.799E-01	17	B200	1 0 0 0 1	
2.255E-03	4.198E-01	20	B200	1 0 0 0 1	
1.179E-02	2.195E+00	20	C092	2 2 0 1 2	
2.228E-03	4.148E-01	25	M061	1 0 0 0 2	average of 2

2767. $C_{12}H_{10}O_2$
2-Hydroxydiphenyl ether
2-Hydroxy-diphenyl-aether
RN: 2417-10-9 **MP** (°C)**:**
MW: 186.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.907E-04	1.100E-01	20	F300	1 0 0 0 1	

2768. $C_{12}H_{10}O_3$
β-Naphthoxyacetic acid
(2-Naphthoxy)acetic acid
Phyomone
BNOA
RN: 120-23-0 **MP** (°C)**:** 155–157
MW: 202.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.330E-04	8.756E-02	25	D088	0 0 0 0 0	
8.100E-04	1.638E-01	35	D088	0 0 0 0 0	
1.100E-05	2.224E-03	45	D088	0 0 0 0 0	

2769. $C_{12}H_{10}O_4$
Quinhydrone
Chinhydron
RN: 106-34-3 **MP** (°C)**:** 171
MW: 218.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.861E-02	4.061E+00	25	B121	1 2 2 1 2	average of 4

2770. $C_{12}H_{11}ClN_2O_5S$
Furosemide
Frusemide
RN: 54-31-9 **MP** (°C)**:** 206
MW: 330.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-05	1.850E-02	20	B405	1 1 1 2 2	
1.814E-05	6.000E-03	22.5	C438	0 0 0 0 0	
1.784E-05	5.900E-03	25	A408	2 0 1 2 0	
2.691E-05	8.900E-03	25	B405	1 1 1 2 2	Buffer pH 2.0
7.559E-05	2.500E-02	25	B405	1 1 1 2 2	
1.875E-05	6.200E-03	25	F415	0 0 0 0 0	Average
2.210E-04	7.310E-02	30	E049	2 0 2 2 2	

(*continued*)

2770. $C_{12}H_{11}ClN_2O_5S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.023E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.778E-05	5.882E-03	ns	R427	0 0 0 0 0	

2771. $C_{12}H_{11}Cl_2NO$

Propyzamide
3,5-Dichloro-*N*-(1,1-dimethyl-2-propynyl)benzamide
Pronamide
Kerb 50W
RH-315

RN: 23950-58-5 **MP** (°C)**:** 155.5
MW: 256.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.856E-05	1.500E-02	25	M161	1 0 0 0 1	

2772. $C_{12}H_{11}I_3N_2O_4$

Iodamide
3-Acetamido-5-acetamidomethyl-2,4,6-triiodobenzoic acid
3-Acetylamino-5-acetylaminomethyl-2,4,6-triiodobenzoic acid
Jodomiron 380
Uromiro
Uromiron

RN: 440-58-4 **MP** (°C)**:**
MW: 627.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.777E-03	3.000E+00	20	F045	1 2 2 2 1	
5.096E-03	3.200E+00	40	F045	1 2 2 2 1	
6.211E-03	3.900E+00	60	F045	1 2 2 2 1	

2773. $C_{12}H_{11}N$

Diphenylamine
4-Aminobiphenyl

RN: 122-39-4 **MP** (°C)**:** 53.5
MW: 169.23 **BP** (°C)**:** 302.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-03	3.079E-01	20	B179	0 0 0 0 0	
3.132E-04	5.300E-02	20	H300	1 2 2 2 1	
3.274E-04	5.540E-02	20	T301	1 2 2 2 2	
2.765E-04	4.680E-02	25	F029	1 0 0 0 2	
3.415E-04	5.780E-02	50	T301	1 2 2 2 2	average of 5
3.557E-04	6.020E-02	80	T301	1 2 2 2 2	average of 5
1.772E-03	2.999E-01	rt	D021	0 0 1 1 0	

2774. $C_{12}H_{11}NO_2$
Fenfuram
2-Methyl-*N*-phenyl-3-furancarboxamide
Pano-ram
RN: 24691-80-3 **MP** (°C)**:** 109.5
MW: 201.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.970E-04	1.000E-01	20	M161	1 0 0 0 0	

2775. $C_{12}H_{11}NO_2$
Carbaryl
1-Naphthyl *N*-methylcarbamate
Devicarb
Hexavin
Karbaspray
Murvin
RN: 63-25-2 **MP** (°C)**:** 142
MW: 201.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	5.453E-02	5	H343	0 0 0 0 0	
3.598E-04	7.239E-02	10	B324	0 0 0 0 0	
3.444E-04	6.930E-02	10	B324	0 0 0 0 0	
3.150E-04	6.339E-02	10	H343	0 0 0 0 0	
3.740E-04	7.526E-02	15	H343	0 0 0 0 0	
1.995E-04	4.015E-02	20	B179	0 0 0 0 0	
5.164E-04	1.039E-01	20	B300	2 1 1 1 2	
4.947E-04	9.955E-02	20	B324	0 0 0 0 0	
5.168E-04	1.040E-01	20	B324	0 0 0 0 0	
2.485E-04	5.000E-02	20	F311	1 2 2 2 1	
4.450E-04	8.955E-02	20	H343	0 0 0 0 0	
1.690E-04	3.400E-02	22	K137	1 1 2 1 0	
1.988E-04	4.000E-02	22.5	G301	0 0 0 0 0	
5.210E-04	1.048E-01	25	H343	0 0 0 0 0	
6.184E-04	1.244E-01	30	B324	0 0 0 0 0	
6.460E-04	1.300E-01	30	B324	0 0 0 0 0	
1.988E-04	4.000E-02	30	D089	2 2 0 0 0	
6.520E-04	1.312E-01	30	H343	0 0 0 0 0	
1.988E-04	4.000E-02	30	M161	1 0 0 0 1	
7.860E-04	1.582E-01	35	H343	0 0 0 0 0	
8.990E-04	1.809E-01	40	H343	0 0 0 0 0	
1.006E-03	2.024E-01	45	H343	0 0 0 0 0	
1.988E-04	4.000E-02	ns	H042	0 0 0 0 1	
2.783E-04	5.600E-02	ns	M110	0 0 0 0 0	EFG

2776. $C_{12}H_{11}N_3$
C.I. Solvent yellow 1
p-Aminoazobenzene
4-Aminoazobenzene
4-Amino-azobenzol
RN: 60-09-3 **MP** (°C)**:** 125
MW: 197.24 **BP** (°C)**:** >360

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.591E-04	1.300E-01	18	F300	1 0 0 0 1	
1.500E-04	2.959E-02	25	B333	0 0 0 0 0	
2.484E-04	4.900E-02	37	H120	1 1 1 1 1	normal saline
5.510E-04	1.087E-01	60	B198	1 2 1 1 2	
1.041E-03	2.053E-01	71.80	B198	1 2 1 1 2	
1.907E-03	3.761E-01	84.10	B198	1 2 1 1 2	
3.431E-03	6.767E-01	97.40	B198	1 2 1 1 2	

2777. $C_{12}H_{11}N_3$
Diazoaminobenzene
1,3-Diphenyltriazene
Anilinoazobenzene
N-(Phenylazo)aniline
RN: 136-35-6 **MP** (°C)**:** 98.0
MW: 197.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-03	4.998E-01	rt	D021	0 0 1 1 0	

2778. $C_{12}H_{11}N_3O_3$
Orotic acid benzylamide
Orotamide, *N*-benzyl-
RN: 13156-36-0 **MP** (°C)**:** 260–263
MW: 245.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-02	1.128E+01	–4	N018	0 0 0 0 0	
8.700E-02	2.134E+01	16	N018	0 0 0 0 0	
1.180E-01	2.894E+01	25	N018	0 0 0 0 0	

2779. $C_{12}H_{11}O_4P$
Diphenyl phosphate
Phosphoric acid, diphenyl ester
RN: 838-85-7 **MP** (°C)**:** 63
MW: 250.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.08E-03	>2.70E-01	24	H116	2 1 0 0 0	

2780. $C_{12}H_{12}$
1,5-Dimethylnaphthalene
RN: 571-61-9 **MP** (°C)**:** 81
MW: 156.23 **BP** (°C)**:** 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.754E-05	2.740E-03	25	E004	2 1 2 2 2	
2.163E-05	3.380E-03	25	M064	1 1 2 2 2	
2.160E-05	3.375E-03	25	M342	1 0 1 1 2	
2.163E-05	3.380E-03	ns	M344	0 0 0 0 2	

2781. $C_{12}H_{12}$
1-Ethylnaphthalene
RN: 1127-76-0 **MP** (°C)**:** –15
MW: 156.23 **BP** (°C)**:** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-05	8.124E-03	10	S076	2 2 2 2 1	
5.200E-05	8.124E-03	14	S076	2 2 2 2 1	
6.400E-05	9.999E-03	20	S076	2 2 2 2 1	
6.849E-05	1.070E-02	25	M064	1 1 2 2 2	
6.850E-05	1.070E-02	25	M342	1 0 1 1 2	
6.400E-05	9.999E-03	25	S076	2 2 2 2 1	
6.849E-05	1.070E-02	ns	M344	0 0 0 0 2	

2782. $C_{12}H_{12}$
2,3-Dimethylnaphthalene
RN: 581-40-8 **MP** (°C)**:** 103
MW: 156.23 **BP** (°C)**:** 269

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.274E-05	1.990E-03	25	E004	2 1 2 2 2	
1.920E-05	3.000E-03	25	M064	1 1 2 2 1	
1.920E-05	3.000E-03	25	M342	1 0 1 1 2	
1.920E-05	3.000E-03	ns	M344	0 0 0 0 1	

2783. $C_{12}H_{12}$
1,3-Dimethylnaphthalene
RN: 575-41-7 **MP** (°C)**:** –5
MW: 156.23 **BP** (°C)**:** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-05	8.000E-03	25	M064	1 1 2 2 1	
5.120E-05	7.999E-03	25	M342	1 0 1 1 2	
5.121E-05	8.000E-03	ns	M344	0 0 0 0 1	

2784. $C_{12}H_{12}$
2,6-Dimethylnaphthalene
RN: 581-42-0 **MP** (°C)**:** 109
MW: 156.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-05	2.000E-03	25	M064	1 1 2 2 1	
1.280E-05	2.000E-03	25	M342	1 0 1 1 2	
1.280E-05	2.000E-03	ns	M344	0 0 0 0 1	

2785. $C_{12}H_{12}$
2-Ethylnaphthalene
RN: 939-27-5 **MP** (°C)**:** –7.4
MW: 156.23 **BP** (°C)**:** 251.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.895E-05	9.210E-03	20	B356	0 0 0 0 0	
5.121E-05	8.000E-03	25	E004	2 1 2 2 2	

2786. $C_{12}H_{12}$
1,4-Dimethylnaphthalene
RN: 571-58-4 **MP** (°C)**:** 7.6
MW: 156.23 **BP** (°C)**:** 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.544E-05	7.100E-03	4	D351	1 2 1 1 2	
4.744E-05	7.412E-03	10	D351	1 2 1 1 2	
6.081E-05	9.500E-03	20	B318	0 0 0 0 0	EFG
6.062E-05	9.470E-03	20	B356	0 0 0 0 0	
6.167E-05	9.634E-03	25	D351	1 2 1 1 2	
7.297E-05	1.140E-02	25	M064	1 1 2 2 2	
7.300E-05	1.140E-02	25	M342	1 0 1 1 1	
7.944E-05	1.241E-02	40	D351	1 2 1 1 2	
7.297E-05	1.140E-02	ns	M344	0 0 0 0 2	

2787. $C_{12}H_{12}ClNO$
2-Chloro-*N*-(1-methyl-2-propynyl)acetanilide
Basamaize
RN: 35846-47-0 **MP** (°C)**:** 40
MW: 221.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	5.000E-01	20	B200	1 0 0 0 0	

2788. $C_{12}H_{12}N_2$
Benzidine
Benzidin
p-Diaminobiphenyl
RN: 92-87-5 **MP** (°C)**:** 117
MW: 184.24 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E-03	3.599E-01	24	H106	1 0 2 2 2	
1.954E-03	3.600E-01	24	M303	1 0 1 1 2	pH 5.9
2.712E-03	4.998E-01	25	B019	1 0 1 2 0	
2.822E-03	5.200E-01	25	B068	2 0 1 1 1	
2.700E-04	4.975E-02	25	H091	1 2 2 2 1	*sic*
1.465E-03	2.699E-01	rt	N015	0 0 2 2 2	

2789. $C_{12}H_{12}N_2$
m-Benzidine
3-Benzidine
RN: 2050-89-7 **MP** (°C)**:** 117
MW: 184.24 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.970E-02	1.100E+01	100	F300	1 0 0 0 1	

2790. $C_{12}H_{12}N_2OS$
2,4-Dimethyl-5-carboxanilidothiazole
G-696
RN: 21452-18-6 **MP** (°C)**:** 141
MW: 232.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-02	2.454E+00	25	M061	1 0 0 0 2	

2791. $C_{12}H_{12}N_2O_2S$
Dapsone
4,4′-Diaminodiphenyl sulphone
RN: 80-08-0 **MP** (°C)**:** 175
MW: 248.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.638E-04	1.400E-01	25	P351	0 0 0 0 0	pH 7.4
6.444E-04	1.600E-01	25	P351	0 0 0 0 0	
1.530E-03	3.800E-01	37	L037	1 2 2 1 1	
4.027E-04	1.000E-01	ns	K444	0 0 0 0 0	

2792. $C_{12}H_{12}N_2O_2S$
Sulfabenz
Sulfanilid
RN: 127-77-5 **MP** (°C)**:**
MW: 248.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.819E-02	7.000E+00	100	F300	1 0 0 0 0	

2793. $C_{12}H_{12}N_2O_3$
Nalidixic acid
NegGRAM
1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid
Nalidic acid
RN: 389-08-2 **MP** (°C)**:** 228
MW: 232.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.306E-04	1.000E-01	23	G098	1 0 0 0 0	
7.079E-01	1.644E+02	37	O307	1 0 1 2 1	pH 2, EFG
4.306E-04	1.000E-01	ns	K444	0 0 0 0 0	

2794. $C_{12}H_{12}N_2O_3$
Phenobarbital
5-Ethyl-5-phenylbarbituric acid
Phenylethylmalonylurea
RN: 50-06-6 **MP** (°C)**:** 176
MW: 232.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-03	9.243E-01	15	H018	0 0 0 0 0	
3.680E-03	8.546E-01	15	S149	1 2 2 1 2	anhydrate

(*continued*)

2794. $C_{12}H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-03	7.385E-01	15	S149	1 2 2 1 2	hydrate
4.736E-03	1.100E+00	20	I009	1 2 2 1 1	EFG, 0.005M HCl
3.789E-03	8.800E-01	20	J030	1 2 2 2 1	
4.521E-03	1.050E+00	20	K143	1 2 2 2 2	form II
5.081E-03	1.180E+00	20	K143	1 2 2 2 2	form III
3.143E-03	7.300E-01	20	N023	1 2 2 1 1	hydrate
4.866E-03	1.130E+00	20	N023	1 2 2 1 2	anhydrate
3.920E-03	9.104E-01	20	S149	1 2 2 1 2	hydrate
4.510E-03	1.047E+00	20	S149	1 2 2 1 2	anhydrate
4.731E-03	1.099E+00	25	A023	1 0 0 1 1	
5.167E-03	1.200E+00	25	B011	2 0 0 1 0	
4.994E-03	1.160E+00	25	B065	1 1 1 1 0	
5.590E-03	1.298E+00	25	E011	2 1 1 2 1	
7.737E-03	1.797E+00	25	E011	2 1 1 2 1	pH 7.0
3.078E-02	7.149E+00	25	E011	2 1 1 2 1	pH 8.0
4.731E-03	1.099E+00	25	F009	2 2 2 2 0	EFG
4.600E-03	1.068E+00	25	G003	1 1 1 1 1	pH 4.7
2.734E-03	6.350E-01	25	H005	1 0 1 2 2	
5.161E-03	1.199E+00	25	K010	2 0 0 1 1	
6.114E-03	1.420E+00	25	K143	1 2 2 2 2	form III
5.512E-03	1.280E+00	25	K143	1 2 2 2 2	form II
4.650E-03	1.080E+00	25	L032	2 1 2 0 2	
4.790E-03	1.112E+00	25	M056	2 2 2 2 2	
5.684E-03	1.320E+00	25	N023	1 2 2 1 2	anhydrate
4.995E-03	1.160E+00	25	N023	1 2 2 1 2	hydrate
6.020E-03	1.398E+00	25	P006	2 0 2 2 1	
4.306E-03	1.000E+00	25	P015	0 0 0 0 0	
4.761E-03	1.106E+00	25	P350	0 0 0 0 0	intrinsic
4.830E-03	1.122E+00	25	S149	1 2 2 1 2	hydrate
5.320E-03	1.236E+00	25	S149	1 2 2 1 2	anhydrate
5.170E-03	1.201E+00	25	V033	2 0 1 1 2	
5.200E-03	1.208E+00	25.00	T303	1 0 0 0 1	
6.700E-03	1.556E+00	30	A065	2 0 2 2 1	
6.310E-03	1.465E+00	30	H018	0 0 0 0 0	
6.000E-03	1.393E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
6.100E-03	1.417E+00	30	K108	1 2 2 0 1	
6.502E-03	1.510E+00	30	K143	1 2 2 2 2	form II
7.148E-03	1.660E+00	30	K143	1 2 2 2 2	form III
6.071E-03	1.410E+00	30	N023	1 2 2 1 2	hydrate
6.502E-03	1.510E+00	30	N023	1 2 2 1 2	anhydrate
6.020E-03	1.398E+00	30	O321	0 0 0 0 0	
6.000E-03	1.393E+00	30	O321	0 0 0 0 0	
8.612E-03	2.000E+00	32	M157	2 0 1 1 0	EFG
7.737E-03	1.797E+00	35	A023	1 0 0 1 2	
7.700E-03	1.788E+00	35	S149	1 2 2 1 2	hydrate
7.750E-03	1.800E+00	35	S149	1 2 2 1 2	anhydrate
8.500E-03	1.974E+00	35.00	T303	1 0 0 0 1	

(*continued*)

2794. $C_{12}H_{12}N_2O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.923E-03	1.840E+00	37	J030	1 2 2 2 2	
8.000E-03	1.858E+00	37	K121	1 2 1 2 0	0.1N HCl
9.023E-03	2.096E+00	40	A023	1 0 0 1 2	
9.000E-02	2.090E+01	40	N008	1 0 1 1 2	*sic*
1.055E-02	2.450E+00	45	S149	1 2 2 1 2	anhydrate
1.108E-02	2.573E+00	45	S149	1 2 2 1 2	hydrate
1.130E-02	2.624E+00	45.00	T303	1 0 0 0 2	
1.266E-02	2.940E+00	50	S149	1 2 2 1 2	anhydrate
1.506E-02	3.498E+00	50	S149	1 2 2 1 2	hydrate
1.698E-02	3.943E+00	55	S149	1 2 2 1 2	hydrate
1.499E-02	3.481E+00	55	S149	1 2 2 1 2	anhydrate
1.033E-02	2.400E+00	60	I009	1 2 2 1 1	EFG, 0.005M HCl
4.306E-03	1.000E+00	ns	K444	0 0 0 0 0	
4.177E-03	9.700E-01	ns	T003	0 0 0 0 2	

2795. $C_{12}H_{12}N_2O_6S_2$
Benzidine-2,2′-disulfonic acid
Benzidin-disulfosaeure-(2,2′)
RN: 117-61-3 **MP** (°C)**:**
MW: 344.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-03	8.000E-01	25	F300	1 0 0 0 0	

2796. $C_{12}H_{12}N_2S$
Thiopyrine
1-Phenyl-2,3-dimethyl-3-pyrazoline-5-thione
RN: 5702-69-2 **MP** (°C)**:** 166
MW: 216.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-02	1.428E+01	ns	D087	0 2 0 0 2	

2797. $C_{12}H_{12}N_4O_3$
Benznidazole
2-Nitro-*N*-(phenylmethyl)-imidazole-1-acetamide
RN: 22994-85-0 **MP** (°C)**:**
MW: 260.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	ns	K444	0 0 0 0 0	

2798. $C_{12}H_{12}N_4O_3S$
*N*4-Acetylsulfapyrazine
*N*4-Acetylsulphapyrazine
RN: 5433-91-0 **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2799. $C_{12}H_{12}N_4O_3S$
*N*4-Acetyl sulfadiazine
*N*4-Acetylsulfadiazine
Acetyl sulfadiazine
2-*N*4-Acetylsulfanilamidopyrimidine
RN: 127-74-2 **MP** (°C)**:**
MW: 292.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
	1.500E-01	37	F075	1 0 2 2 2	
7.200E-04	2.105E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
6.842E-04	2.000E-01	37	L091	1 0 0 0 1	pH 5.5
8.723E-04	2.550E-01	37	M057	1 0 0 0 2	pH 5.5
5.131E-04	1.500E-01	37	R045	1 2 1 1 1	

2800. $C_{12}H_{12}N_6O_6$
TMPPT
1,3,7,9-Tetramethylpyrimido(5,4-γ) pteridine-2,4,6,8(1H,3H,7H,9H)-tetrone
RN: **MP** (°C)**:**
MW: 336.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-04	1.298E-01	25	K008	1 1 0 1 0	EFG
3.900E-04	1.311E-01	25	K009	1 2 1 1 0	EFG

2801. $C_{12}H_{12}O_6$
Benzoic acid, 2-(acetyloxy)-, (acetyloxy)methyl ester
Salicylic acid acetate, hydroxymethyl ester acetate
RN: 32620-68-1 **MP** (°C)**:** oil
MW: 252.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.634E-03	2.430E+00	21	N335	0 0 0 0 0	

2802. $C_{12}H_{13}ClN_2O$
Buturon
3-(*para*-Chlorophenyl)-1-methyl-1-(1-methyl-2-propynyl) urea
Urea, *N′*-(4-chlorophenyl)-*N*-methyl-*N*-(1-methyl-2-propynyl)
Eptapur
RN: 3766-60-7 **MP** (°C)**:** 145.5
MW: 236.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.267E-04	3.000E-02	20	G036	1 0 0 0 1	
1.267E-04	3.000E-02	20	M161	1 0 0 0 1	

2803. $C_{12}H_{13}ClN_4$
Pyrimethamine
RN: 58-14-0 **MP** (°C)**:** 238
MW: 248.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E-05	1.000E-02	ns	K444	0 0 0 0 0	

2804. $C_{12}H_{13}I_3N_2O_2$
Iopodic acid
Ipodic acid
RN: 5587-89-3 **MP** (°C)**:**
MW: 597.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.027E-03	1.810E+00	ns	H055	0 0 0 0 0	

2805. $C_{12}H_{13}I_3N_2O_3$
Iocetamic acid
N-(3-Amino-2,4,6-triiodophenyl)-3-acetamido-2-methylpropionic acid
Cholebrine
MP 620
DRC 1201
RN: 16034-77-8 **MP** (°C)**:** 224
MW: 613.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.610E-03	5.286E+00	37	J016	1 0 0 0 2	pH 7.4

2806. $C_{12}H_{13}NO_2$
Methsuximide
Celontin
N-Methyl-α-methyl-α-phenylsuccinimide
RN: 77-41-8 **MP** (°C)**:** 52–53
MW: 203.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.378E-02	2.800E+00	25	P061	0 0 0 0 0	

2807. $C_{12}H_{13}NO_2S$
Carboxin
2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin
Vitavax
RN: 5234-68-4 **MP** (°C)**:** 94
MW: 235.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.225E-04	1.700E-01	25	M061	1 0 0 0 2	
7.225E-04	1.700E-01	25	M161	1 0 0 0 2	

2808. $C_{12}H_{13}NO_2S$
4-Thiazolidinecarboxylic acid, 2-(4-ethenylphenyl)-
RN: 256235-52-6 **MP** (°C)**:**
MW: 235.31 **BP** (°C)**:** 464.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	8.706E-01	21	B414	1 0 0 1 1	partial decomposition

2809. $C_{12}H_{13}NO_3$
Azetidine, 1-[(benzoyloxy)acetyl]-
RN: 115178-66-0 **MP** (°C)**:** 74.5
MW: 219.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-02	5.400E+00	22	N317	1 1 2 1 2	

2810. $C_{12}H_{13}NO_3$
Crotonyl acetaminophen
Crotonic acid, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, crotonate (ester)
RN: 20675-24-5 **MP** (°C)**:** 146-147
MW: 219.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.961E-03	4.300E-01	37	D029	0 0 0 0 0	

2811. $C_{12}H_{13}NO_4$
Acetamide, *N*-acetyl-2-(benzoyloxy)-*N*-methyl-
RN: 115178-80-8 **MP** (°C)**:**
MW: 235.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	N317	1 1 2 1 2	

2812. $C_{12}H_{13}NO_4S$
Plantvax
2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin-4,4-dioxide
Oxycarboxin
RN: 5259-88-1 **MP** (°C)**:** 128.7
MW: 267.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.741E-03	1.000E+00	25	M161	1 0 0 0 0	
3.741E-03	1.000E+00	ns	M061	0 0 0 0 2	

2813. $C_{12}H_{13}NO_4S_2$
4-Ethylsulfonylnaphthalene-1-sulfonamide
ENS
4-ENS
RN: 842-00-2 **MP** (°C)**:**
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.775E-04	1.130E-01	c	K042	2 2 2 2 2	

2814. $C_{12}H_{13}NO_5$
Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-
RN: 106231-64-5 **MP** (°C)**:** 160.5
MW: 251.24 **BP** (°C)**:** 475.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.572E-03	1.400E+00	22	B427	1 0 0 1 1	in 0.01M HCl
5.572E-03	1.400E+00	22	N317	1 1 2 1 2	

2815. $C_{12}H_{13}NO_5$
Succinyl acetaminophen
Butanedioic acid, mono[4-(acetylamino)phenyl] ester
Acetanilide, 4′-hydroxy-, hydrogen succinate ester
RN: 20675-25-6 **MP** (°C)**:** 145.5-146.5
MW: 251.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-02	6.500E+00	37	D029	0 0 0 0 0	

2816. $C_{12}H_{13}NO_6$
Carbobenzoxydiglycine
RN: **MP** (°C)**:**
MW: 267.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-03	6.500E-01	25.1	N026	0 0 0 0 0	
2.804E-03	7.494E-01	25.1	N027	1 1 2 2 2	

2817. $C_{12}H_{13}N_3O_2$
Isocarboxazid
Marplan
RN: 59-63-2 **MP** (°C)**:**
MW: 231.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-03	8.000E-01	25	R024	0 0 0 0 0	

2818. $C_{12}H_{13}N_3O_2S$
*N*1-Methyl-*N*1-2-pyridyl-sulfanilamide
*N*1-Methyl-*N*1-(2-pyridyl)sulfanilamide
RN: 51543-29-4 **MP** (°C)**:**
MW: 263.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.740E-03	1.248E+00	37	K095	2 0 0 0 2	intrinsic

2819. $C_{12}H_{13}N_3O_3S_2$
Methyl acetyl sulfathiazole
Sulfathiazol methyle acetyle
RN: **MP** (°C)**:**
MW: 311.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.248E-04	7.000E-02	37	D084	1 0 1 0 0	

2820. $C_{12}H_{13}N_3O_4S$
Acetylsulfamethoxazole
Acetanilide, 4′-[(5-methyl-3-isoxazolyl)sulfamoyl]-
4′-Acetyl-3-sulfa-5-methylisoxazole
RN: 21312-10-7 **MP** (°C)**:**
MW: 295.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.573E-04	7.600E-02	37	H120	1 1 1 1 1	normal saline

2821. $C_{12}H_{14}ClNO_2$
Clomazone
Command
Dimethazone
Fenoxan
FMC 57020
Gamit
RN: 81777-89-1 **MP** (°C)**:** 25
MW: 239.70 **BP** (°C)**:** 275.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.101E+00	ns	S460	0 0 0 0 0	

2822. $C_{12}H_{14}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-butyl ester
2,4-Dichlorophenoxyacetic acid butyl ester
RN: 94-80-4 **MP** (°C)**:**
MW: 277.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.495E-05	1.523E-02	ns	M120	0 0 1 1 2	

2823. $C_{12}H_{14}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *sec*-butyl ester

RN: 94-79-1 **MP** (°C)**:**
MW: 277.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.252E-05	1.733E-02	ns	M120	0 0 1 1 2	

2824. $C_{12}H_{14}Cl_3O_4P$

Chlorfenvinphos
2-Chloro-1-(2,4-dichlorophenyl)ethenyl phosphoric acid, diethyl ester
Dermaton
Birlanex
Birlane
Steladone

RN: 470-90-6 **MP** (°C)**:**
MW: 359.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
4.074E-04	1.465E-01	20	B179	0 0 0 0 0	
3.449E-04	1.240E-01	20	B300	2 1 1 1 2	
3.449E-04	1.240E-01	20	B324	0 0 0 0 0	
3.448E-04	1.240E-01	20	B324	0 0 0 0 0	
3.893E-04	1.400E-01	20	F311	1 2 2 2 1	
4.033E-04	1.450E-01	20	M061	1 0 0 0 2	
4.033E-04	1.450E-01	23	M161	1 0 0 0 2	
2.976E-04	1.070E-01	30	B324	0 0 0 0 0	
2.975E-04	1.070E-01	30	B324	0 0 0 0 0	

2825. $C_{12}H_{14}NO_4PS$

Ditalimfos
O,*O*-Diethyl (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl) phosphonothioate
Laptran
Plondrel

RN: 5131-24-8 **MP** (°C)**:** 83.5
MW: 299.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.444E-04	1.330E-01	rt	M161	0 0 0 0 2	

2826. $C_{12}H_{14}N_2O_2$
Primidone
5-Ethyldihydro-5-phenyl-4,6(1H,5H)-pyrimidinedione
Desoxyphenobarbitone
2-Deoxyphenobarbital
RN: 125-33-7 **MP** (°C)**:** 281.5
MW: 218.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-03	4.700E-01	25	C437	0 0 0 0 0	Average
2.200E-03	4.802E-01	30	K108	1 2 2 0 1	
2.747E-03	5.996E-01	37	P061	0 0 0 0 0	
2.291E-03	5.000E-01	rt	D025	0 0 0 0 0	

2827. $C_{12}H_{14}N_2O_4$
Acetamide, *N*-(2-amino-2-oxoethyl)-2-(benzoyloxy)-*N*-methyl-
RN: 106231-62-3 **MP** (°C)**:** 101.5
MW: 250.26 **BP** (°C)**:** 496.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-01	3.020E+01	22	B427	1 0 0 1 1	in 0.01M HCl
1.207E-01	3.020E+01	22	N317	1 1 2 1 2	

2828. $C_{12}H_{14}N_2O_4$
Propanamide, 2-[[(benzoyloxy)acetyl]amino]-
RN: 115193-30-1 **MP** (°C)**:** 201.5
MW: 250.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	4.800E-01	22	N317	1 1 2 1 2	

2829. $C_{12}H_{14}N_2O_5$
2-Cyclohexyl-4,6-dinitrophenol
Dinex
4,6-Dinitro-2-cyclohexylphenol
2,4-Dinitro-6-cyclohexylphenol
RN: 131-89-5 **MP** (°C)**:** 106
MW: 266.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.634E-05	1.500E-02	25	M061	1 0 0 0 1	pH 6.5
6.760E-06	1.800E-03	25	M061	1 0 0 0 1	pH 1

2830. $C_{12}H_{14}N_2O_6$
Dinoseb acetate
Aretit
RN: 2813-95-8 **MP** (°C)**:** 26.5
MW: 282.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.794E-03	2.200E+00	rt	M161	0 0 0 0 1	

2831. $C_{12}H_{14}N_4O_2S$
6-Sulfanilamido-2,4-dimethylpyrimidine
6-Sulfanilamido-2,4-dimethylpyrimidin
Sulfisomidine
Sulphasomidine
RN: 515-64-0 **MP** (°C)**:** 243.0
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.965E-03	1.382E+00	25	M319	2 1 1 1 2	
6.862E-03	1.910E+00	37	K086	1 0 0 0 2	
5.802E-03	1.615E+00	ns	B133	0 2 0 1 2	pH 7.4
1.075E-02	2.991E+00	ns	M141	0 0 0 0 0	

2832. $C_{12}H_{14}N_4O_2S$
Sulfamethazine
Sulfadimezine
2-Sulfanilamido-4,6,-dimethylpyrimidine
RN: 57-68-1 **MP** (°C)**:** 176
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.317E-03	1.480E+00	20	F073	1 2 2 2 2	
1.544E-03	4.298E-01	20	L058	1 0 1 1 2	
1.893E-03	5.269E-01	20	O032	1 0 0 0 2	
1.424E-03	3.963E-01	24	N021	2 0 1 2 2	pH 5.6
1.600E-03	4.453E-01	25	M440	0 0 0 0 0	
5.389E-03	1.500E+00	29	C049	0 0 0 0 0	
2.695E-03	7.500E-01	37	L091	1 0 0 0 1	pH 5.5
6.862E-03	1.910E+00	37	M057	1 0 0 0 2	pH 5.5
2.414E-03	6.720E-01	37	S192	1 0 1 1 2	pH 6.0
2.299E-03	6.400E-01	38	K006	1 0 0 0 1	
1.185E-03	3.299E-01	ns	L044	0 0 0 0 2	

2833. $C_{12}H_{14}N_4O_2S.0.5H_2O$
Sulphamethazine (hemihydrate)
Sulfamethazine hemihydrate
RN: 57-68-1 **MP** (°C)**:**
MW: 287.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.786E-03	1.950E+00	37	R044	0 0 0 0 0	

2834. $C_{12}H_{14}N_4O_2S$
2-Sulfanilamido-4,5-dimethylpyrimidine
RN: 4462-43-5 **MP** (°C)**:** 225.7
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.186E-04	2.000E-01	29	C049	0 0 0 0 0	

2835. $C_{12}H_{14}N_4O_2S$
2-Sulfanilylamino-4-ethylpyrimidine
RN: 2276-96-2 **MP** (°C)**:**
MW: 278.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.180E-04	1.720E-01	37	R076	1 2 0 0 2	

2836. $C_{12}H_{14}N_4O_3S_2$
Acetyl sulfaethylthiadiazole
Acetamide, *N*-[4-[[(5-ethyl-1,3,4-thiadiazol-2-yl)amino]sulfonyl]phenyl]-
RN: 1037-51-0 **MP** (°C)**:**
MW: 326.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E-03	1.620E+00	37	B046	1 0 2 2 2	pH 4.6

2837. $C_{12}H_{14}N_4O_3S$
Sulfamethomidine
Sulphamethomidine
RN: 3772-76-7 **MP** (°C)**:** 146.0
MW: 294.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.864E-03	8.430E-01	ns	B133	0 2 0 1 2	pH 7.4
2.884E-03	8.489E-01	ns	R427	0 0 0 0 0	

2838. $C_{12}H_{14}N_4O_3S$
2-Sulfanilamido-4-ethoxypyrimidine
RN: 71138-72-2 **MP** (°C)**:**
MW: 294.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-04	5.300E-02	37	R046	1 2 1 1 2	

2839. $C_{12}H_{14}N_4O_4S$
Sulfadimethoxine
Sulphadimethoxine
RN: 122-11-2 **MP** (°C)**:** 202.0
MW: 310.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.492E-04	4.630E-02	37	W055	1 2 0 1 2	
1.105E-03	3.430E-01	ns	B133	0 2 0 1 2	pH 7.4

2840. $C_{12}H_{14}N_4O_4S$
Sulfadoxine
Sulformethoxine
Sulforthomidine
4-Amino-*N*-(5,6-dimethoxy-4-pyrimidinyl)benzenesulfonamide
Fanzil
Fanasil
RN: 2447-57-6 **MP** (°C)**:** 190–194
MW: 310.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.761E-04	2.098E-01	ns	R427	0 0 0 0 0	

2841. $C_{12}H_{14}O_4$
Diethyl phthalate
Ethyl phthalate
Di-ethyl phthalate
Phthalic acid ethyl ester
Phthalsaeure-diaethyl ester
RN: 84-66-2 **MP** (°C)**:** –40.5
MW: 222.24 **BP** (°C)**:** 296.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.495E-03	9.990E-01	20	F070	1 0 0 0 0	
4.180E-03	9.290E-01	20	L300	2 1 0 2 2	
1.793E-02	3.984E+00	20.00	D343	0 0 0 0 0	
5.399E-03	1.200E+00	25	F067	1 0 2 2 2	
4.500E-03	1.000E+00	25	F300	1 0 0 0 0	

2842. $C_{12}H_{14}O_4$
Trimethylacetyl salicylate
Salicylic acid, pivalate
2-Carboxyphenyl pivalate
RN: 2704-58-7 **MP** (°C)**:**
MW: 222.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.730E-04	2.162E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.74, intrinsic

2843. $C_{12}H_{14}O_4$
Diethyl *o*-phthalate
RN: **MP** (°C)**:** –40 C
MW: 222.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-03	8.040E-01	25	S417	0 0 0 0 0	

2844. $C_{12}H_{15}ClNO_4PS_2$
Phosalone
Diethyl *S*-((6-chloro-2-oxobenzoxazolin-3-yl)methyl) phosphorodithioate
Rubitox
Benzophosphate
RN: 2310-17-0 **MP** (°C)**:**
MW: 367.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B300	2 2 1 1 2	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
5.845E-06	2.150E-03	20	C053	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
5.845E-06	2.150E-03	ns	F071	0 1 2 1 2	
2.719E-05	1.000E-02	rt	M161	0 0 0 0 1	

2845. $C_{12}H_{15}ClO_3$
Clofibrate
2-(*p*-Chlorophenoxy)-2-methylpropionic acid ethyl ester
Abitrate
Atromid S
RN: 637-07-0 **MP** (°C)**:**
MW: 242.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.708E-02	rt	G093	0 1 1 1 2	

2846. $C_{12}H_{15}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-propanoate
5′-Propionyl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-propionate
RN: 84043-25-4 **MP** (°C)**:** 167.5
MW: 410.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E+03	1.427E+06	25	N332	0 0 0 0 0	pH 7.4

2847. $C_{12}H_{15}NO$
n-Propylcinnamamide
Cinnamamide, *N*-propyl-
2-Propenamide, 3-phenyl-*N*-propyl-
RN: 6329-15-3 **MP** (°C)**:**
MW: 189.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.353E-01	ns	H350	0 0 0 0 0	

2848. $C_{12}H_{15}NO_3$
Acetamide, *N*-[2-(benzoyloxy)ethyl]-*N*-methyl-
RN: 57440-16-1 **MP** (°C)**:**
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	3.130E+01	22	N317	1 1 2 1 2	

2849. $C_{12}H_{15}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-propyl-
RN: 106231-51-0 **MP** (°C)**:** 89.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.893E-03	6.400E-01	22	B427	1 0 0 1 1	in 0.01M HCl
2.893E-03	6.400E-01	22	N317	1 1 2 1 2	

2850. $C_{12}H_{15}NO_3$
Propanamide, 3-(benzoyloxy)-*N*,*N*-dimethyl-
RN: 115178-77-3 **MP** (°C)**:**
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.955E-02	1.760E+01	22	N317	1 1 2 1 2	

2851. $C_{12}H_{15}NO_3$
Carbofuran
2,3-Dihydro-2,2-dimethyl-7-benzofuranol methylcarbamate
Crisfuran
Furadanx
Curaterr
RN: 1563-66-2 **MP** (°C)**:** 152
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-03	2.909E-01	10	B324	0 0 0 0 0	
1.315E-03	2.910E-01	10	B324	0 0 0 0 0	
1.446E-03	3.199E-01	19	B169	2 1 1 1 1	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
3.164E-03	7.000E-01	25	M161	1 0 0 0 2	
1.695E-03	3.750E-01	30	B324	0 0 0 0 0	
1.694E-03	3.749E-01	30	B324	0 0 0 0 0	
1.446E-03	3.200E-01	ns	V414	0 0 0 0 0	

2852. $C_{12}H_{15}NO_3$
Acetaminophen butyrate
Butyryl acetaminophen
Butanoic acid, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, butyrate
RN: 14771-98-3 **MP** (°C)**:** 140
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	3.300E-01	25	B010	1 1 1 1 0	
2.441E-03	5.400E-01	37	D029	0 0 0 0 0	

2853. $C_{12}H_{15}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-(1-methylethyl)-
RN: 115193-27-6 **MP** (°C)**:** 129.5
MW: 221.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-03	4.100E-01	22	N317	1 1 2 1 2	

2854. $C_{12}H_{15}NO_4$
Isopropyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl 1-methylethyl ester
Acetanilide, 4′-hydroxy-, isopropyl carbonate
RN: 17239-27-9 **MP** (°C)**:** 131.5–132
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.636E-03	1.100E+00	37	D029	0 0 0 0 0	

2855. $C_{12}H_{15}NO_4$
Acetamide, 2-(benzoyloxy)-*N*-(2-hydroxyethyl)-*N*-methyl-
RN: 106231-59-8 **MP** (°C)**:** 79
MW: 237.26 **BP** (°C)**:** 428.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.135E-02	1.930E+01	22	B427	1 0 0 1 1	in 0.01M HCl
8.135E-02	1.930E+01	22	N317	1 1 2 1 2	

2856. $C_{12}H_{15}NO_4$
O-(Butyryloxymethyl) salicylamide
O-Butyryloxymethyl salicylamide
Butanoic acid, [2-(aminocarbonyl)phenoxy]methyl ester
RN: 103951-39-9 **MP** (°C)**:** 57
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	2.500E+00	23	B328	1 2 2 1 1	pH 4.0
1.054E-02	2.500E+00	23	B328	0 0 0 0 0	

2857. $C_{12}H_{15}NO_5$
Benzoic acid, 2-hydroxy-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl ester
N-Methyl-*N*-carbamoylmethyl glycolamide salicylate
RN: 114665-09-7 **MP** (°C)**:** 92.5
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.300E+00	21	B331	1 2 2 1 0	pH 7.4
2.488E-02	6.300E+00	21	B331	0 0 0 0 0	

2858. $C_{12}H_{15}NO_6$
Ethonyphenyl tartramic acid
RN: **MP** (°C)**:** 201
MW: 269.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.989E+00	14	C069	1 2 0 1 2	

2859. $C_{12}H_{15}N_2O_3PS$
Phoxim
4-Ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile 4-sulfide
Baythion
Sebacil
Volation
RN: 14816-18-3 **MP** (°C)**:**
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-05	3.300E-03	10	B324	0 0 0 0 0	
1.106E-05	3.299E-03	10	B324	0 0 0 0 0	
1.374E-05	4.099E-03	20	B300	2 1 1 1 2	
1.374E-05	4.099E-03	20	B324	0 0 0 0 0	
1.374E-05	4.100E-03	20	B324	0 0 0 0 0	

(*continued*)

2859. $C_{12}H_{15}N_2O_3PS$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-05	7.000E-03	20	M161	1 0 0 0 0	
1.643E-05	4.901E-03	30	B324	0 0 0 0 0	
1.643E-05	4.900E-03	30	B324	0 0 0 0 0	
1.374E-05	4.099E-03	ns	S460	0 0 0 0 0	

2860. $C_{12}H_{15}N_2O_3PS$

Quinalphos
Diethyl *O*-(2-quinoxalyl) phosphorothioate
Diethquinalphion
Bayrusil
Ekalux

RN: 13593-03-8 **MP** (°C)**:** 33.5
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.375E-05	2.200E-02	24	M161	1 0 0 0 1	

2861. $C_{12}H_{15}N_3O_2S$

1-Methyl-2-sulfanilamide-1,2-dihydropyridine
Benzenesulfonamide, 4-amino-*N*-(1,2-dihydro-1-methyl-2-pyridinyl)-

RN: 51543-30-7 **MP** (°C)**:**
MW: 265.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-03	9.791E-01	37	K095	2 0 0 0 2	intrinsic

2862. $C_{12}H_{15}N_3O_2S$

Albendazole
Bilutac
Eskazole
Proftril
Valbazan
Zentel

RN: 54965-21-8 **MP** (°C)**:**
MW: 265.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-06	7.500E-04	209	D426	0 0 0 0 0	
3.769E-05	1.000E-02	ns	K444	0 0 0 0 0	

2863. $C_{12}H_{15}N_3O_3$
Triallyl cyanurate
Cyanursaeure-triallylaether
RN: 101-37-1 **MP** (°C)**:** 26–28
MW: 249.27 **BP** (°C)**:** 119–120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.407E-02	6.000E+00	20	F300	1 0 0 0 0	

2864. $C_{12}H_{15}N_3O_3S$
Albendazole sulphoxide
Ricobendazole
Albendazole oxide
Methoxy-*N*-[5-(propylsulfinyl)benzimidazol-2-yl]carboxamide
Albendazole oxide [BAN:INN]
Carbamic acid
RN: 54029-12-8 **MP** (°C)**:**
MW: 281.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.204E-04	6.200E-02	25	W416	0 0 0 0 0	
1.094E-03	3.079E-01	94.1	D426	0 0 0 0 0	

2865. $C_{12}H_{15}N_3O_6$
1,3,5-Triglycidyl-*S*-triazinetrione
α-TGT
RN: 2451-62-9 **MP** (°C)**:**
MW: 297.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.373E-02	1.300E+01	0	A088	0 0 1 1 1	

2866. $C_{12}H_{15}N_5O_5$
9-[5′-(*O*-Acetyl)-β-D-arabinofuranosyl]adenine ester
Vidarabine 5′-acetate
RN: 65926-28-5 **MP** (°C)**:** 198.0
MW: 309.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.134E-02	6.600E+00	ns	B134	0 1 1 1 1	

2867. $C_{12}H_{15}N_5O_5$
Pivaloyl salicylate
9-(2-*O*-Acetyl-β-D-arabinofuranosyl)adenine
RN: 87970-03-4 **MP** (°C)**:** 195
MW: 309.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-01	9.360E+01	37	B306	1 2 0 1 2	pH 7.3

2868. $C_{12}H_{15}O_3P$
Diallyl phenyl phosphonate
Phosphonic acid, phenyl-, di-2-propenyl ester
RN: 2948-89-2 **MP** (°C)**:**
MW: 238.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-03	3.000E-01	25	B070	1 2 0 1 0	

2869. $C_{12}H_{16}ClNOS$
Orbencarb
Lanray
S-((2-Chlorophenyl)methyl) diethylcarbamothioate
RN: 34622-58-7 **MP** (°C)**:**
MW: 257.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-05	2.400E-02	ns	S460	0 0 0 0 0	

2870. $C_{12}H_{16}ClNOS$
Thiobencarb
S-4-Chlorobenzyl diethylthiocarbamate
Diethylcarbamothioic acid *S*-[(4-chlorophenyl)methyl] ester
4-Chlorobenzyl *N*,*N*-diethylthiocarbamate
RN: 28249-77-6 **MP** (°C)**:**
MW: 257.78 **BP** (°C)**:** 127.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-04	3.000E-02	22	K137	1 1 2 1 0	
1.164E-04	3.001E-02	ns	S460	0 0 0 0 0	

2871. $C_{12}H_{16}Cl_2N_2O$
Neburon
1-Butyl-3-(3,4-dichlorophenyl)-1-methylurea
RN: 555-37-3 **MP** (°C)**:** 101.5
MW: 275.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.744E-05	4.800E-03	20	F311	1 2 2 2 1	
1.744E-05	4.800E-03	24	B185	0 0 0 0 0	
1.744E-05	4.800E-03	24	G036	1 0 0 0 1	
1.744E-05	4.800E-03	24	M061	1 0 0 0 1	
1.744E-05	4.800E-03	24	M161	1 0 0 0 1	
1.744E-05	4.800E-03	25	A039	1 1 0 0 1	
1.744E-05	4.800E-03	25	G099	1 0 0 1 0	
1.744E-05	4.800E-03	ns	K007	0 0 0 0 1	

2872. $C_{12}H_{16}N_2$
Etryptamine
α-Ethyltryptamine
RN: 2235-90-7 **MP** (°C)**:** 97
MW: 188.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.709E-03	5.100E-01	rt	M011	0 0 2 1 1	intrinsic

2873. $C_{12}H_{16}N_2O$
N-(Piperidinomethyl)benzamide
Benzamide, *N*-(1-pyrrolidinylmethyl)-
RN: 92788-60-8 **MP** (°C)**:**
MW: 204.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-03	1.450E+00	22	J037	0 0 0 0 0	

2874. $C_{12}H_{16}N_2O_2$
N,*N*,*N*′,*N*′-Tetramethylterephthalamide
1,4-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 13158-31-1 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.843E+00	4.060E+02	30	K004	1 0 0 0 2	
1.840E+00	4.053E+02	30	K019	1 0 0 0 2	

2875. $C_{12}H_{16}N_2O_2$

N,*N*,*N*′,*N*′-Tetramethylphthalamide
1,2-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 6329-16-4 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.223E+00	7.100E+02	30	K004	1 0 0 0 2	

2876. $C_{12}H_{16}N_2O_2$

N,*N*,*N*′,*N*′-Tetramethylisophthalamide
1,3-Benzenedicarboxamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 14334-36-2 **MP** (°C)**:**
MW: 220.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E+00	6.760E+02	30	K004	1 0 0 0 2	
3.070E+00	6.762E+02	30	K019	1 0 0 0 2	

2877. $C_{12}H_{16}N_2O_2S$

4-Thiazolidinecarboxylic acid, 2-[4-(dimethylamino)phenyl]-
4-Thiazolidinecarboxylic acid, 2-(*p*-dimethylaminophenyl)-
RN: 72678-86-5 **MP** (°C)**:**
MW: 252.34 **BP** (°C)**:** 481.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.813E-01	21	B414	1 0 0 1 1	fast decomposition

2878. $C_{12}H_{16}N_2O_3$

Hexobarbital
5-(1-Cyclohexen-1-yl)-1,5-dimethylbarbituric acid
5-(1-Cyclohexenyl)-1,5-dimethylbarbituric acid
Hexabarital
RN: 56-29-1 **MP** (°C)**:** 146
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-03	2.900E-01	20	J030	1 2 2 2 1	
1.840E-03	4.347E-01	25	M056	2 2 2 2 2	
2.000E-03	4.725E-01	30	K108	1 2 2 0 1	
2.709E-03	6.400E-01	37	J030	1 2 2 2 1	

2879. $C_{12}H_{16}N_2O_3$
Carbetamide
N-Ethyl-2-(((phenylamino)carbonyl)oxy)propanamide
Leguarme
RN: 16118-49-3 **MP** (°C)**:** >110
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.500E+00	20	M161	1 0 0 0 1	

2880. $C_{12}H_{16}N_2O_3$
Cyclobarbital
Phanodorm
RN: 52-31-3 **MP** (°C)**:** 173
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.772E-03	1.600E+00	20	F300	1 0 0 0 1	
6.941E-03	1.640E+00	20	J030	1 2 2 2 2	
3.500E-02	8.270E+00	25	G003	1 1 1 1 1	pH 4.7
8.000E-03	1.890E+00	30	G014	1 1 1 1 0	EFG
7.800E-03	1.843E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
8.000E-03	1.890E+00	30	K108	1 2 2 0 1	
9.735E-03	2.300E+00	37	F300	1 0 0 0 1	
9.523E-03	2.250E+00	37	J030	1 2 2 2 2	
9.140E-02	2.160E+01	40	N008	1 2 1 1 2	*sic*

2881. $C_{12}H_{16}N_3O_3PS$
Triazophos
O,*O*-Diethyl *O*-(1-phenyl-1H-1,2,4-triazol-3-yl) phosphorothioate
Hostathion
RN: 24017-47-8 **MP** (°C)**:**
MW: 313.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.884E-05	2.470E-02	20	B300	2 1 1 1 2	
1.245E-04	3.900E-02	23	M161	1 0 0 0 1	
1.245E-04	3.900E-02	23	T305	1 0 0 0 1	
1.245E-04	3.899E-02	ns	S460	0 0 0 0 0	

2882. $C_{12}H_{16}N_3O_3PS_2$
Azinphos-ethyl
O,*O*-Diethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
Azinos
Ethyl guthion
RN: 2642-71-9 **MP** (°C)**:**
MW: 345.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B300	2 2 1 1 2	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
7.152E-05	2.470E-02	30	B324	0 0 0 0 0	
7.151E-05	2.470E-02	30	B324	0 0 0 0 0	
3.020E-05	1.043E-02	ns	R427	0 0 0 0 0	

2883. $C_{12}H_{16}N_4O_2$
2,5-Diaziridinyl-3,6-bis(methylamino)-1,4-benzoquinone
Benzoquinone-2,5-bisaziridinyl-3,6-bismethyl amino
RN: 59886-52-1 **MP** (°C)**:** 220
MW: 248.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.03E-04	<1.00E-01	rt	C317	0 0 0 0 0	

2884. $C_{12}H_{16}N_4O_2S_2$
Glybuthiazole
p-Aminobenzenesulfamido-*tert*-butylthiodiazole
Glipasol
Glypasol
RN: 535-65-9 **MP** (°C)**:** 222
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	5.686E-02	37	A046	2 0 1 1 2	

2885. $C_{12}H_{16}N_4O_2S_2$
4-Amino-*N*-(5-butyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Sulfanilamide, *N*1-(5-butyl-1,3,4-thiadiazol-2-yl)-
RN: 71119-31-8 **MP** (°C)**:**
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	8.466E-02	37	A046	2 0 1 1 2	

2886. $C_{12}H_{16}N_4O_7S$
2′-Methylsulfonyl-6-methoxypurine arabinoside
9H-Purine, 6-methoxy-9-[2-*O*-(methylsulfonyl)-β-D-arabinofuranosyl]-
RN: 145913-48-0 **MP** (°C)**:** 188-190
MW: 360.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-02	6.198E+00	37	C348	0 0 0 0 0	pH 7.00

2887. $C_{12}H_{16}N_5O_3PS_2$
Azinphos-ethyl *O*-analog
RN: **MP** (°C)**:**
MW: 373.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-02	3.797E+00	10	B300	2 2 1 1 2	

2888. $C_{12}H_{16}O$
o-Cyclohexylphenol
2-Cyclohexylphenol
RN: 119-42-6 **MP** (°C)**:**
MW: 176.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.727E-04	8.333E-02	25	L021	1 0 0 0 0	

2889. $C_{12}H_{16}O$
p-Cyclohexylphenol
4-Cyclohexylphenol
RN: 1131-60-8 **MP** (°C)**:**
MW: 176.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.782E-04	6.666E-02	25	L021	1 0 0 0 0	

2890. $C_{12}H_{16}O_2$
ε-Phenylcaproic acid
6-Phenylcaproic acid
6-Phenylhexanoic acid
RN: 5581-75-9 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-03	4.798E-01	30	D033	2 2 1 2 2	
4.002E-03	7.694E-01	40	D033	2 2 1 2 2	

2891. $C_{12}H_{16}O_2$
4-Cyclohexylresorcinol
p-Cyclohexylresorcinol
RN: 2138-20-7 **MP** (°C)**:**
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-03	4.998E-01	25	L021	1 0 0 0 0	

2892. $C_{12}H_{16}O_3$
Isoamyl salicylate
Isoamyl *o*-hydroxybenzoate
3-Methylbutyl salicylate
3-Methylbutyl *o*-hydroxybenzoate
RN: 87-20-7 **MP** (°C)**:**
MW: 208.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.961E-04	1.450E-01	25	D081	1 2 2 1 2	
6.918E-04	1.441E-01	ns	S460	0 0 0 0 0	

2893. $C_{12}H_{16}O_7.H_2O$
Arbutin (monohydrate)
Hydroquinone-β-D-glucopyranoside monohydrate
RN: 6058-77-1 **MP** (°C)**:** 195–200
MW: 290.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.828E-01	1.111E+02	c	D004	0 0 0 0 0	
1.723E+00	5.000E+02	h	D004	0 0 0 0 0	

2894. $C_{12}H_{17}NO_2$
2,6-Diethyl-4-acetaminophenol
3,5-Diethylparacetamol
4-Acetamido-2,6-diethylphenol
RN: 55205-89-5 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-03	6.101E-01	25	D078	1 2 1 1 2	

2895. $C_{12}H_{17}NO_2$
Promecarb
5-Isopropyl-*m*-tolyl methylcarbamate
Carbamult
RN: 2631-37-0 **MP** (°C)**:** 87.5
MW: 207.27 **BP** (°C)**:** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-04	9.200E-02	rt	M161	0 0 0 0 1	

2896. $C_{12}H_{17}NO_2$
Pentyl *p*-aminobenzoate
4-Aminobenzoic acid pentyl ester
RN: 13110-37-7 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	8.084E-02	37	F006	1 1 2 2 1	
1.890E-04	3.917E-02	ns	M066	0 0 0 0 2	
1.890E-04	3.917E-02	rt	B016	0 0 1 1 2	pH 7.4

2897. $C_{12}H_{17}NO_2$
2-*sec*-Butylphenyl methylcarbamate
BPMC
2-(1-Methylpropyl)phenol methylcarbamate
N-Methyl *O*-*sec*-butylphenylcarbamate
RN: 3766-81-2 **MP** (°C)**:** 32
MW: 207.27 **BP** (°C)**:** 112.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.294E-04	8.900E-02	22	K137	1 1 2 1 0	
3.184E-03	6.600E-01	30	M161	1 0 0 0 2	

2898. $C_{12}H_{17}NO_2$
Hexyl nicotinate
n-Hexyl nicotinoate
Nicotinic acid *n*-hexyl ester
RN: 23597-82-2 **MP** (°C)**:**
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.202E-04	1.700E-01	32	L346	1 0 0 1 2	

2899. $C_{12}H_{17}NO_2$
m-tert-Butylphenyl *N*-methylcarbamate
3-*tert*-Butylphenyl *N*-methylcarbamate
RN: 780-11-0 **MP** (°C)**:** 144.0
MW: 207.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.41E-06	<5.00E-04	30	D089	2 2 0 0 0	

2900. $C_{12}H_{17}NO_3$
m-sec-Butoxyphenyl *N*-methylcarbamate
3-*sec*-Butoxyphenyl *N*-methylcarbamate
RN: 13538-22-2 **MP** (°C)**:** 53
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-04	8.000E-02	30	D089	2 2 0 0 0	

2901. $C_{12}H_{17}NO_3$
m-n-Butoxyphenyl *N*-methylcarbamate
3-*n*-Butoxyphenyl *N*-methylcarbamate
RN: 3978-68-5 **MP** (°C)**:** 54.5
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.000E-02	30	D089	2 2 0 0 0	

2902. $C_{12}H_{17}NO_3$
Acetamide, *N*-[4-(1-ethoxyethoxy)phenyl]-
1-(*p*-Acetaminophenoxy)-1-ethoxyethane
RN: 51736-24-4 **MP** (°C)**:**
MW: 223.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.698E-01	ns	H076	0 0 0 0 0	

2903. $C_{12}H_{17}NO_4$
3,5-Dimethoxy-acetophenetide
RN: **MP** (°C)**:**
MW: 239.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.904E-01	1.173E+02	21.80	B102	2 0 1 1 1	solid hydrate
3.344E+00	8.000E+02	35.60	B102	2 0 1 1 2	liquid hydrate
8.778E-01	2.100E+02	39.40	B102	2 0 1 1 1	solid hydrate

(*continued*)

2903. $C_{12}H_{17}NO_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E+00	7.736E+02	45.60	B102	2 0 1 1 2	liquid hydrate
1.586E+00	3.795E+02	57	B102	2 0 1 1 1	solid hydrate
3.172E+00	7.591E+02	58.10	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	68.50	B102	2 0 1 1 2	liquid hydrate
2.100E+00	5.026E+02	69.50	B102	2 0 1 1 1	solid hydrate
2.288E+00	5.474E+02	72.80	B102	2 0 1 1 1	solid hydrate
2.569E+00	6.147E+02	77.10	B102	2 0 1 1 2	solid hydrate
2.790E+00	6.675E+02	80.20	B102	2 0 1 1 2	solid hydrate
2.947E+00	7.053E+02	82.60	B102	2 0 1 1 2	solid hydrate
3.049E+00	7.296E+02	84.20	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	84.30	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	86	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	86.90	B102	2 0 1 1 2	solid hydrate
3.348E+00	8.011E+02	99.80	B102	2 0 1 1 2	liquid hydrate
3.459E+00	8.275E+02	111.10	B102	2 0 1 1 2	liquid hydrate
3.527E+00	8.440E+02	118.40	B102	2 0 1 1 2	liquid hydrate
3.632E+00	8.690E+02	129.20	B102	2 0 1 1 2	liquid hydrate
4.031E+00	9.645E+02	173.60	B102	2 0 1 1 2	liquid hydrate

2904. $C_{12}H_{17}N_2O_2$

4-Aminobenzoic acid-2-(propyl-amino)ethyl ester
2-(Propylamino)ethyl 4-aminobenzoate
4-Aminobenzoic acid 2-(propyl-amino)ethyl ester

RN: **MP** (°C)**:**
MW: 221.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	6.638E-02	ns	M066	0 0 0 0 0	

2905. $C_{12}H_{17}N_3O_4S$

3′-Nitroso-tolbutamide

RN: **MP** (°C)**:**
MW: 299.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.341E-04	1.000E-01	25	G051	1 0 1 1 0	

2906. $C_{12}H_{17}N_5O_3$

N,*N*-Diethylglycyloxymethyl-1-allopurinol
Glycine, *N*,*N*-diethyl-, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98204-08-1 **MP** (°C)**:**
MW: 279.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-02	4.500E+00	22	B323	0 0 0 0 0	

2907. $C_{12}H_{17}O_4PS_2$
Phenthoate
Dimethyl-*S*-(α-ethoxycarbonylbenzyl) phosphorodithioate
Elsan
Fenthoate
Phent
Cidial
RN: 2597-03-7 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-04	2.000E-01	20	M161	1 0 0 0 2	
3.434E-05	1.100E-02	22	K137	1 1 2 1 0	
3.119E-05	9.992E-03	ns	S460	0 0 0 0 0	

2908. $C_{12}H_{18}$
1-Phenylhexane
Hexylbenzene
n-Hexylbenzene
RN: 1077-16-3 **MP** (°C)**:** –61
MW: 162.28 **BP** (°C)**:** 226

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-06	9.214E-04	5.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	6.04	M183	1 2 1 1 2	
5.140E-06	8.341E-04	7	O312	2 2 0 2 2	
5.667E-06	9.196E-04	8.04	M183	1 2 1 1 2	
5.583E-06	9.060E-04	9.04	M183	1 2 1 1 2	
5.150E-06	8.357E-04	10	O312	2 2 0 2 2	
5.572E-06	9.042E-04	10.04	M183	1 2 1 1 2	
5.717E-06	9.277E-04	11.04	M183	1 2 1 1 2	
5.733E-06	9.304E-04	12.04	M183	1 2 1 1 2	
5.667E-06	9.196E-04	13.04	M183	1 2 1 1 2	
5.700E-06	9.250E-04	14.04	M183	1 2 1 1 2	
5.090E-06	8.260E-04	15	O312	2 2 0 2 2	
5.594E-06	9.079E-04	15.04	M183	1 2 1 1 2	
5.661E-06	9.187E-04	16.04	M183	1 2 1 1 2	
5.606E-06	9.097E-04	17.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	18.04	M183	1 2 1 1 2	
5.811E-06	9.430E-04	19.04	M183	1 2 1 1 2	
5.860E-06	9.509E-04	20	O312	2 2 0 2 2	
5.850E-06	9.493E-04	20.04	M183	1 2 1 1 2	
5.889E-06	9.556E-04	21.04	M183	1 2 1 1 2	
5.872E-06	9.529E-04	22.04	M183	1 2 1 1 2	
6.056E-06	9.827E-04	23.04	M183	1 2 1 1 2	
6.133E-06	9.953E-04	24.04	M183	1 2 1 1 2	
6.270E-06	1.017E-03	25	M342	1 0 1 1 2	
5.560E-06	9.023E-04	25	O312	2 2 0 2 2	

(*continued*)

2908. $C_{12}H_{18}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.156E-06	9.989E-04	25.04	M183	1 2 1 1 2	
6.156E-06	9.989E-04	26.04	M183	1 2 1 1 2	
6.239E-06	1.012E-03	27.04	M183	1 2 1 1 2	
6.261E-06	1.016E-03	29.04	M183	1 2 1 1 2	
6.140E-06	9.964E-04	30	O312	2 2 0 2 2	
6.590E-06	1.069E-03	35	O312	2 2 0 2 2	
6.590E-06	1.069E-03	40	O312	2 2 0 2 2	
8.000E-06	1.298E-03	45	O312	2 2 0 2 2	
2.000E-03	3.246E-01	ns	H307	0 0 0 0 0	

2909. $C_{12}H_{18}N_2O$

Isoproturon
N,*N*-Dimethyl-*N′*-(4-(1-methylethyl)phenyl)urea
3-(4-Isopropylphenyl)-1,1-dimethylurea
Tolkan
DPX 6774

RN: 34123-59-6 **MP** (°C)**:** 158.5
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.909E-04	6.000E-02	20	M161	1 0 0 0 1	

2910. $C_{12}H_{18}N_2O_2$

Zectran
4-Dimethylamino-3,5-dimethylphenol methylcarbamate ester
Mexacarbole
Mexacarbate

RN: 315-18-4 **MP** (°C)**:** 85
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E-04	9.999E-02	25	I314	0 0 0 0 0	

2911. $C_{12}H_{18}N_2O_2S$

Thiamylal
5-Allyl-5-(1-methyl-butyl)-barbituric acid
5-Allyl-5-(1-methylbutyl)-2-thiobarbituric acid

RN: 77-27-0 **MP** (°C)**:** 132
MW: 254.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.104E-03	1.298E+00	25	A023	1 0 0 1 1	
1.966E-04	5.000E-02	25	B011	2 0 0 1 0	
1.944E-04	4.946E-02	25	B065	1 1 1 1 2	

(*continued*)

2911. $C_{12}H_{18}N_2O_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-04	8.852E-02	25	G003	1 1 1 1 1	pH 4.7
7.500E-03	1.908E+00	30	G014	1 1 1 1 0	EFG
6.600E-03	1.679E+00	30	I001	2 0 2 1 0	EFG, 0.003N H_2SO_4
8.630E-03	2.195E+00	40	A023	1 0 0 1 1	
3.750E-03	9.538E-01	40	N008	1 2 1 1 2	*sic*
8.792E-03	2.236E+00	ns	G039	0 0 0 0 0	EFG

2912. $C_{12}H_{18}N_2O_3$

5-Isopropyl-5-(3-methylbut-2-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methyl-2-butenyl)-5-(1-methylethyl)
5-*i*-Propyl-5-(3-methylbut-2-enyl)barbiturate

RN: 67051-26-7 **MP** (°C)**:**
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-03	6.088E-01	25	P350	0 0 0 0 0	intrinsic

2913. $C_{12}H_{18}N_2O_3$

Secobarbital
5-Allyl-5-(1-methylbutyl)barbituric acid
Seconal

RN: 76-73-3 **MP** (°C)**:** 98
MW: 238.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.250E-03	1.728E+00	25	G003	1 1 1 1 2	pH 7
4.410E-03	1.051E+00	25	V033	2 0 1 1 2	
4.400E-03	1.048E+00	25.00	T303	1 0 0 0 1	
6.300E-03	1.501E+00	35.00	T303	1 0 0 0 1	
7.900E-02	1.882E+01	40	N008	1 0 1 1 2	*sic*
9.400E-03	2.240E+00	45.00	T303	1 0 0 0 1	

2914. $C_{12}H_{18}N_2O_3S$

Tolbutamide
1-Butyl-3-(*para*-tolylsulfonyl) urea
Oramide
Orinase

RN: 64-77-7 **MP** (°C)**:** 129
MW: 270.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.178E-04	1.400E-01	25	G051	1 0 1 1 0	
4.068E-04	1.100E-01	25	P096	0 0 0 0 0	

(*continued*)

2914. $C_{12}H_{18}N_2O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.054E-01	30	G318	0 0 0 0 0	EFG
4.027E-04	1.089E-01	37	A028	1 0 2 1 2	intrinsic
4.030E-04	1.090E-01	37	A046	2 0 1 1 2	
5.659E-04	1.530E-01	37	B138	1 2 0 0 2	pH 1.5, form II
5.289E-04	1.430E-01	37	B138	1 2 0 0 2	pH 1.5, form III
5.067E-04	1.370E-01	37	B138	1 2 0 0 2	pH 1.5, form I
3.699E-04	1.000E-01	37.0	H033	1 0 2 1 0	pH 1.4, intrinsic
3.031E-03	8.193E-01	37.5	F015	1 0 2 2 1	pH 6.0, pKa 5.32
2.535E-02	6.853E+00	37.5	F015	1 0 2 2 2	pH 7.0, pKa 5.32

2915. $C_{12}H_{18}N_2O_4S$

Anisylbutamide
Methoxyphenylbutazolamide
Methoxytolbutamide

RN: 24535-67-9 **MP** (°C)**:**
MW: 286.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.236E-04	1.213E-01	37	A028	1 0 2 1 2	intrinsic
4.260E-04	1.220E-01	37	A046	2 0 1 1 2	

2916. $C_{12}H_{18}N_2O_5$

D-Mannosephenylhydrazone
D-Mannose-phenylhydrazon

RN: 6147-14-4 **MP** (°C)**:** 195.5
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.811E-02	1.030E+01	100	F300	1 0 0 0 2	

2917. $C_{12}H_{18}N_4O_6S$

Oryzalin
3,5-Dinitro-*N*4,*N*4-dipropylsulfanilamide

RN: 19044-88-3 **MP** (°C)**:** 137
MW: 346.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-04	8.500E-02	25	B200	1 0 0 0 1	
6.929E-06	2.400E-03	25	M161	1 0 0 0 1	

2918. $C_{12}H_{18}O$
Propofol
2,6-Diisopropylphenol
Diisopropylphenol
Diprivan
RN: 2078-54-8 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.975E-04	1.600E-01	amb	L434	0 0 0 0 0	

2919. $C_{12}H_{18}O$
2-Butyl-4-ethylphenol
Phenol, 2-butyl-4-ethyl-
RN: 3781-74-6 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2920. $C_{12}H_{18}O$
2-Butyl-4,6-dimethylphenol
2,6-Xylenol, 2-butyl-
RN: 6483-60-9 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L020	1 0 0 0 0	

2921. $C_{12}H_{18}O$
o-*n*-Hexylphenol
2-*n*-Hexylphenol
RN: 3226-32-2 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L022	1 0 0 0 0	

2922. $C_{12}H_{18}O$
2-Butyl-4,5-dimethylphenol
Phenol, 2-butyl-4,5-dimethyl-
RN: **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2923. $C_{12}H_{18}O$
2-Butyl-6-ethylphenol
Phenol, 2-butyl-6-ethyl-
RN: 22496-45-3 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2924. $C_{12}H_{18}O$
2,6-Dipropylphenol
Phenol, 2,6-dipropyl-
RN: 6626-32-0 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2925. $C_{12}H_{18}O$
4-Butyl-2,5-dimethylphenol
2,5-Xylenol, 4-butyl-
RN: 91763-77-8 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2926. $C_{12}H_{18}O$
4-Butyl-2,6-dimethylphenol
Phenol, 4-butyl-2,6-dimethyl-
2,6-Xylenol, 4-butyl-
RN: 6676-26-2 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2927. $C_{12}H_{18}O$
p-*n*-Hexylphenol
4-*n*-Hexylphenol
RN: 2446-69-7 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L022	1 0 0 0 0	

2928. $C_{12}H_{18}O$
2,4-Dipropylphenol
Phenol, 2,4-dipropyl-
RN: 23167-99-9 **MP** (°C)**:**
MW: 178.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2929. $C_{12}H_{18}O_2$
4-Hexylresorcinol
4-*n*-Hexylresorcin
RN: 136-77-6 **MP** (°C)**:** 68
MW: 194.28 **BP** (°C)**:** 334

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.574E-03	5.000E-01	18	F300	1 0 0 0 1	

2930. $C_{12}H_{18}O_4S_2$
Di-isopropyl 1,3-dithiolan-2-ylidinemalonate
Isoprothiolane
Fuji-one
bis(1-Methylethyl) 1,3-dithiolan-2-ylidenepropanedioate
RN: 50512-35-1 **MP** (°C)**:** 52.25
MW: 290.40 **BP** (°C)**:** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	4.800E-02	20	H309	0 0 0 0 0	
1.653E-04	4.800E-02	20	M161	1 0 0 0 1	

2931. $C_{12}H_{19}BrN_2O_2$
Neostigmine bromide
Neostigmine bromide
Neostigmine;
Prostigmin
RN: 114-80-7 **MP** (°C)**:**
MW: 303.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.298E+00	1.000E+03	ns	K444	0 0 0 0 0	

2932. $C_{12}H_{19}ClNO_3P$
Crufomate
O-Methyl *O*-2-chloro-4-*tert*-butyphenyl *N*-methylamidophosphate
RN: 299-86-5 **MP** (°C)**:** 60.25
MW: 291.72 **BP** (°C)**:** 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-02	4.975E+00	ns	M061	0 0 0 0 0	

2933. $C_{12}H_{19}N_3O_8$
Orotic acid methylglucamide
RN: **MP** (°C)**:** 184–186
MW: 333.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-01	1.490E+02	–4	N018	0 0 0 0 0	
7.090E-01	2.363E+02	16	N018	0 0 0 0 0	
8.150E-01	2.716E+02	25	N018	0 0 0 0 0	

2934. $C_{12}H_{19}N_6OP$
Triamiphos
5-Amino-1-(bis(dimethylamino)phosphoryl)-3-phenyl-1,2,4-triazole
Triamifos
Wepsyn 155
Wepsyn
bis(Dimethylamino)-(3-amino-5-phenyl-1,2,4-triazol-1-yl)-phosphine oxide
RN: 1031-47-6 **MP** (°C)**:** 167.5
MW: 294.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.495E-04	2.500E-01	20	M161	1 0 0 0 2	

2935. $C_{12}H_{19}O_2PS_3$
Sulprofos
O-Ethyl *O*-[4-(methylthio)phenyl]phosphorodithioic acid *S*-propyl ester
Morpafos
Bolstar
Heliothion
Merdafos
RN: 35400-43-2 **MP** (°C)**:**
MW: 322.45 **BP** (°C)**:** 155–158

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.616E-07	3.101E-04	ns	S460	0 0 0 0 0	

2936. $C_{12}H_{20}$
Triisobutene
1,8-Nonadiene, 2,8-dimethyl-5-methylene-
RN: 36370-80-6 **MP** (°C)**:**
MW: 164.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.944E-08	8.123E-06	20	B165	1 0 1 1 1	
5.838E-03	9.591E-01	97.30	B165	1 0 1 1 1	

2937. $C_{12}H_{20}N_2O_3$
5-Ethyl-5-*n*-hexylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-hexyl-
Hexethal
Ortal
Ortol
RN: 77-30-5 **MP** (°C)**:**
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.930E-04	2.146E-01	25	M310	2 2 2 2 2	

2938. $C_{12}H_{20}N_4O_2$
3-Cyclohexyl-6-dimethylamino-1-methyl-1,3,5-triazine-2,4-dione
1,3,5-Triazine-2,4(1H,3H)-dione, 3-cyclohexyl-6-(dimethylamino)-1-methyl-
Hexazinone
Pronone
DPX 3674
RN: 51235-04-2 **MP** (°C)**:** 116
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.308E-01	3.300E+01	25	M161	1 0 0 0 1	

2939. $C_{12}H_{20}N_4O_6$
Acetyltetraglycine ethyl ester
Glycine, *N*-acetylglycylglycylglycyl-, ethyl ester
RN: 637-83-2 **MP** (°C)**:** 264
MW: 316.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-04	2.600E-01	0	R036	0 0 0 0 0	
2.466E-03	7.800E-01	25	R036	0 0 0 0 0	
5.216E-03	1.650E+00	40	R036	0 0 0 0 0	

2940. $C_{12}H_{20}O_2$
Linalyl acetate
Bergamol
3,7-Dimethyl-1,6-octadien-3-yl acetate
Linalyl
RN: 115-95-7 **MP** (°C)**:**
MW: 196.29 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.546E-03	4.998E-01	25	M350	1 0 1 1 1	

2941. $C_{12}H_{20}O_4$
Dibutyl maleate
Di-*n*-butyl maleate
RN: 105-76-0 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.073E-03	2.450E-01	25	F067	1 0 2 2 2	

2942. $C_{12}H_{20}O_6$
Tripropionin
1,2,3-Propanetriol, tripropanoate
1,2,3-Propanetriyl tripropionate
Tripropionylglycerol
Tripropanoylglycerol
RN: 139-45-7 **MP** (°C)**:**
MW: 260.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-02	3.120E+00	ns	F014	0 0 0 0 2	

2943. $C_{12}H_{21}NO_8S$
Topiramate
2,3:4,5-di-*O*-isopropylidene-β-D-fructopyranose sulfamate
Topamax
Tracrium
RN: 97240-79-4 **MP** (°C)**:**
MW: 339.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-02	9.705E+00	ns	S469	0 0 0 0 0	

2944. $C_{12}H_{21}N_2O_3PS$

Diazinon
O,*O*-Diethyl *O*-(2-isopropyl-6-methyl-4-pyrimidinyl), phosphorothioate
Dimpylate
Basudin
Spectracide
Fezudin

RN: 333-41-5 **MP** (°C)**:** >120
MW: 304.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.336E-04	7.109E-02	10	B324	0 0 0 0 0	
2.336E-04	7.110E-02	10	B324	0 0 0 0 0	
1.318E-04	4.012E-02	20	B179	0 0 0 0 0	
2.261E-04	6.881E-02	20	B300	2 1 1 1 2	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.314E-04	4.000E-02	20	M061	1 0 0 0 1	
2.260E-04	6.880E-02	22	B169	2 1 1 1 2	
1.331E-04	4.050E-02	22	K137	1 1 2 1 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.314E-04	4.000E-02	rt	M161	0 0 0 0 1	

2945. $C_{12}H_{21}N_5O_2S_2$

Nizatidine
Axid
N-(2-(((2-((Dimethylamino)methyl)-4-thiazolyl)methyl)thio)ethyl)-*N′*-methyl-2-nitro-1,1-ethenediamine

RN: 76963-41-2 **MP** (°C)**:**
MW: 331.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.457E-02	2.140E+01	ns	R427	0 0 0 0 0	

2946. $C_{12}H_{21}N_7O$

1-(4′-Formyl-1-piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine
1-Piperazinecarboxaldehyde, 4-[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]-

RN: 126974-79-6 **MP** (°C)**:**
MW: 279.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.670E-03	1.025E+00	25	B386	0 0 0 0 0	

2947. $C_{12}H_{22}N_2O_2$
N,*N*,*N*′,*N*′-Tetraethylfumaramide
2-Butenediamide, *N*,*N*,*N*′,*N*′-tetraethyl-
RN: 111328-65-5 **MP** (°C)**:**
MW: 226.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	1.562E+02	30	K019	1 0 0 0 1	

2948. $C_{12}H_{22}N_6$
1-(Piperidinyl)-3,5-bis(dimethylamino)-*s*-triazine
s-Triazine, 2,4-bis(dimethylamino)-6-piperidino-
RN: 16268-79-4 **MP** (°C)**:**
MW: 250.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	4.402E-02	25	B386	0 0 0 0 0	

2949. $C_{12}H_{22}O_2$
Arbanol
RN: 7070-15-7 **MP** (°C)**:**
MW: 198.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	3.020E-01	6	P430	0 0 0 0 0	
2.911E-03	5.773E-01	23.5	P430	0 0 0 0 0	

2950. $C_{12}H_{22}O_4$
Ethylene glycol divalerate
RN: **MP** (°C)**:**
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.460E-04	1.488E-01	25	F064	1 0 0 0 2	

2951. $C_{12}H_{22}O_4$
1,10-Decanedicarboxylic acid
Decan-dicarbonsaeure-(1,10)
Dodecanedioc acid
RN: 693-23-2 **MP** (°C)**:** 128
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	4.000E-02	20	F300	1 0 0 0 0	
3.039E-03	7.000E-01	21	B040	1 0 1 1 0	*sic*
5.124E-03	1.180E+00	100	F300	1 0 0 0 2	

2952. $C_{12}H_{22}O_4$
Dibutyl succinate
Succinic acid di-*n*-butyl ester
Tabutrex
RN: 141-03-7 **MP** (°C)**:** –29
MW: 230.31 **BP** (°C)**:** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.984E-04	2.299E-01	ns	F014	0 0 0 0 1	

2953. $C_{12}H_{22}O_6$
Triethylene glycol dipropionate
Ethanol, 2,2′-[1,2-ethanediylbis(oxy)]*bis*-, dipropanoate
RN: 141-34-4 **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.394E-01	6.279E+01	ns	F014	0 0 0 0 2	

2954. $C_{12}H_{22}O_6$
Dibutyl tartrate
(2R,3R)-Di-*n*-butyl tartrate
ENT 396
RN: 87-92-3 **MP** (°C)**:** 21
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.840E-02	4.827E+00	ns	F014	0 0 0 0 2	

2955. $C_{12}H_{22}O_6$
Dimethoxyethyl adipate
RN: **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.338E-02	1.400E+01	ns	F014	0 0 0 0 2	

2956. $C_{12}H_{22}O_{11}$
Maltose
D-Glucose, 4-*O*-α-D-glucopyranosyl-
α-Maltose
Malt sugar
RN: 69-79-4 **MP** (°C)**:** 102.5
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.166E-01	2.453E+02	0	C401	1 0 0 0 0	EFG
1.061E+00	3.631E+02	0	M043	1 0 0 0 1	
1.151E+00	3.939E+02	10	M043	1 0 0 0 1	
9.066E-01	3.103E+02	20	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	20	D041	1 0 0 0 2	
1.280E+00	4.382E+02	20	M043	1 0 0 0 1	
1.408E+00	4.819E+02	30	M043	1 0 0 0 1	
1.124E+00	3.846E+02	40	C401	1 0 0 0 0	EFG
1.037E+00	3.548E+02	40	C401	1 0 0 0 0	EFG
1.530E+00	5.238E+02	40	M043	1 0 0 0 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.859E+00	6.364E+02	60	M043	1 0 0 0 2	
1.298E+00	4.444E+02	80	C401	1 0 0 0 0	EFG
2.191E+00	7.500E+02	80	M043	1 0 0 0 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	rt	D021	0 0 1 1 2	

2957. $C_{12}H_{22}O_{11}$
β-Lactose
B-Lactose
Milchzucker
4-*O*-β-D-Galactopyranosyl-D-glucose
RN: 5965-66-2 **MP** (°C)**:** 253
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.525E-01	5.220E+01	20	F300	1 0 0 0 2	
7.303E-02	2.500E+01	h	F300	0 0 0 0 1	

2958. $C_{12}H_{22}O_{11}$
Cellobiose
4-*O*-β-D-Glucopyranosyl-D-glucose
4-β-D-Glucopyransoyl-D-glucopyranose
D-(+)-Cellobiose
RN: 528-50-7 **MP** (°C)**:**
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.243E-01	1.110E+02	15	F300	1 0 0 0 2	
3.475E-01	1.189E+02	30.50	M137	2 1 2 2 2	
1.198E+00	4.100E+02	h	F300	0 0 0 0 1	

2959. $C_{12}H_{22}O_{11}$
Lactose
4-*O*-B-D-Galactopyranosyl-D-glucose
Milk sugar
RN: 63-42-3 **MP** (°C)**:** 201
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.656E-01	9.091E+01	0	C401	1 0 0 0 0	EFG
3.177E-01	1.087E+02	0	M043	1 0 0 0 2	
3.116E-01	1.067E+02	0	P052	1 0 2 2 2	
4.701E-01	1.609E+02	1	P049	1 0 1 1 1	
3.811E-01	1.304E+02	10	M043	1 0 0 0 2	
4.351E-01	1.489E+02	20	C401	1 0 0 0 0	EFG
4.767E-01	1.632E+02	20	M043	1 0 0 0 2	
5.189E-01	1.776E+02	25	D041	1 0 0 0 2	
5.470E-01	1.873E+02	25	P049	1 0 1 1 1	
6.000E-01	2.054E+02	30	D011	1 0 1 0 1	
5.880E-01	2.013E+02	30	M043	1 0 0 0 2	
5.843E-01	2.000E+02	40	C401	1 0 0 0 0	EFG
7.298E-01	2.498E+02	40	M043	1 0 0 0 2	
7.574E-01	2.593E+02	60	C401	1 0 0 0 0	EFG
1.067E+00	3.651E+02	60	M043	1 0 0 0 2	
9.738E-01	3.333E+02	80	C401	1 0 0 0 0	EFG
1.475E+00	5.050E+02	80	M043	1 0 0 0 2	
1.699E+00	5.816E+02	89	D041	1 0 0 0 2	
1.096E+00	3.750E+02	95	C401	1 0 0 0 0	EFG
1.124E+00	3.846E+02	100	C401	1 0 0 0 0	EFG
1.767E+00	6.047E+02	100	M043	1 0 0 0 2	
4.775E-01	1.635E+02	rt	D021	0 0 1 1 2	

2960. $C_{12}H_{22}O_{11}$
Sucrose
Saccharose
β-D-Fructofuranosyl-α-D-glucopyranoside
α-D-Glucopyranosyl β-D-fructofuranoside
Beet sugar
Cane sugar
RN: 57-50-1 **MP** (°C)**:** 191
MW: 342.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E+00	3.902E+02	0	C401	1 0 0 0 0	EFG
1.878E+00	6.429E+02	0	D041	1 0 0 0 2	
1.876E+00	6.421E+02	0	G046	1 0 1 1 2	
1.142E+00	3.909E+02	0	H094	1 0 0 0 2	
1.874E+00	6.416E+02	0	M043	1 0 0 0 2	
1.884E+00	6.450E+02	0	P052	1 0 2 2 2	
1.880E+00	6.435E+02	.90	M074	1 0 0 0 2	average of 3
1.157E+00	3.961E+02	10	H094	1 0 0 0 2	
1.914E+00	6.552E+02	10	M043	1 0 0 0 2	
1.943E+00	6.650E+02	12.5	F300	1 0 0 0 2	
1.938E+00	6.633E+02	15	D041	1 0 0 0 2	
1.934E+00	6.622E+02	15.80	M074	1 0 0 0 2	average of 3
1.931E+00	6.609E+02	18.5	W013	1 2 1 1 2	
1.177E+00	4.030E+02	20	C401	1 0 0 0 0	EFG
1.203E+00	4.118E+02	20	C401	1 0 0 0 0	EFG
1.946E+00	6.660E+02	20	F300	1 0 0 0 2	
1.170E+00	4.005E+02	20	G060	1 0 0 0 2	
1.173E+00	4.015E+02	20	H094	1 0 0 0 2	
1.960E+00	6.711E+02	20	M043	1 0 0 0 2	
1.956E+00	6.697E+02	23.9	W013	1 2 1 1 2	
1.954E+00	6.689E+02	24.4	W013	1 2 1 1 2	
1.964E+00	6.723E+02	24.9	W013	1 2 1 1 2	
1.986E+00	6.798E+02	25	G046	1 0 1 1 2	
1.179E+00	4.036E+02	25	G060	1 0 0 0 2	
1.981E+00	6.779E+02	25.60	M074	1 0 0 0 2	average of 3
1.963E+00	6.721E+02	25.9	W013	1 2 1 1 2	
1.188E+00	4.067E+02	30	G060	1 0 0 0 2	
1.190E+00	4.072E+02	30	H094	1 0 0 0 2	
2.006E+00	6.865E+02	30	M043	1 0 0 0 2	
1.997E+00	6.836E+02	30.0	W013	1 2 1 1 2	
1.996E+00	6.831E+02	30.5	W013	1 2 1 1 2	
2.003E+00	6.855E+02	30.50	M074	1 0 0 0 2	average of 3
2.008E+00	6.873E+02	31.5	W013	1 2 1 1 2	
2.005E+00	6.862E+02	33.1	W013	1 2 1 1 2	
2.025E+00	6.932E+02	34.5	W013	1 2 1 1 2	
2.030E+00	6.950E+02	35	G046	1 0 1 1 2	
1.198E+00	4.100E+02	35	G060	1 0 0 0 2	
2.028E+00	6.942E+02	36.0	W013	1 2 1 1 2	
2.028E+00	6.941E+02	36.4	W013	1 2 1 1 2	
1.252E+00	4.286E+02	40	C401	1 0 0 0 0	EFG

(*continued*)

2960. $C_{12}H_{22}O_{11}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E+00	4.133E+02	40	G060	1 0 0 0 2	
1.207E+00	4.132E+02	40	H094	1 0 0 0 2	
2.057E+00	7.041E+02	40	M043	1 0 0 0 2	
2.050E+00	7.017E+02	40.2	W013	1 2 1 1 2	
2.052E+00	7.023E+02	40.7	W013	1 2 1 1 2	
2.055E+00	7.035E+02	41.0	W013	1 2 1 1 2	
2.061E+00	7.055E+02	42.2	W013	1 2 1 1 2	
2.067E+00	7.074E+02	42.3	W013	1 2 1 1 2	
2.080E+00	7.120E+02	45	F300	1 0 0 0 2	
1.217E+00	4.167E+02	45	G060	1 0 0 0 2	
2.093E+00	7.163E+02	46.1	W013	1 2 1 1 2	
2.107E+00	7.212E+02	49.6	W013	1 2 1 1 2	
2.111E+00	7.225E+02	50	G046	1 0 1 1 2	
1.228E+00	4.202E+02	50	G060	1 0 0 0 2	
7.596E+00	2.600E+03	50	H063	1 0 0 0 2	
1.225E+00	4.194E+02	50	H094	1 0 0 0 2	
2.101E+00	7.191E+02	50.2	W013	1 2 1 1 2	
2.118E+00	7.251E+02	51.1	W013	1 2 1 1 2	
2.124E+00	7.272E+02	52.2	W013	1 2 1 1 2	
2.126E+00	7.276E+02	52.6	W013	1 2 1 1 2	
2.134E+00	7.304E+02	53.6	W013	1 2 1 1 2	
2.134E+00	7.305E+02	53.8	W013	1 2 1 1 2	
2.126E+00	7.278E+02	54.1	W013	1 2 1 1 2	
1.237E+00	4.235E+02	55	G060	1 0 0 0 2	
2.137E+00	7.316E+02	55.8	W013	1 2 1 1 2	
2.147E+00	7.350E+02	56.1	W013	1 2 1 1 2	
2.154E+00	7.372E+02	56.4	W013	1 2 1 1 2	
2.151E+00	7.364E+02	57.5	W013	1 2 1 1 2	
2.154E+00	7.374E+02	57.8	W013	1 2 1 1 2	
2.152E+00	7.368E+02	58.4	W013	1 2 1 1 2	
2.165E+00	7.410E+02	58.6	W013	1 2 1 1 2	
2.166E+00	7.415E+02	59.7	W013	1 2 1 1 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.248E+00	4.273E+02	60	G060	1 0 0 0 2	
1.244E+00	4.259E+02	60	H094	1 0 0 0 2	
2.167E+00	7.416E+02	60	M043	1 0 0 0 2	
2.176E+00	7.448E+02	61.1	W013	1 2 1 1 2	
2.176E+00	7.447E+02	61.4	W013	1 2 1 1 2	
2.182E+00	7.469E+02	62.6	W013	1 2 1 1 2	
2.189E+00	7.493E+02	62.9	W013	1 2 1 1 2	
2.193E+00	7.505E+02	64.6	W013	1 2 1 1 2	
1.258E+00	4.307E+02	65	G060	1 0 0 0 2	
2.204E+00	7.543E+02	65.5	W013	1 2 1 1 2	
2.214E+00	7.580E+02	66.4	W013	1 2 1 1 2	
2.219E+00	7.595E+02	66.5	W013	1 2 1 1 2	
2.222E+00	7.607E+02	68.2	W013	1 2 1 1 2	
2.221E+00	7.603E+02	69.0	W013	1 2 1 1 2	
1.269E+00	4.344E+02	70	G060	1 0 0 0 2	

(*continued*)

2960. $C_{12}H_{22}O_{11}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E+00	7.632E+02	70.1	W013	1 2 1 1 2	
2.233E+00	7.645E+02	70.4	W013	1 2 1 1 2	
2.251E+00	7.706E+02	72.8	W013	1 2 1 1 2	
2.249E+00	7.698E+02	73.8	W013	1 2 1 1 2	
2.267E+00	7.760E+02	74.5	W013	1 2 1 1 2	
2.265E+00	7.752E+02	74.6	W013	1 2 1 1 2	
2.256E+00	7.724E+02	75	G046	1 0 1 1 2	
1.280E+00	4.380E+02	75	G060	1 0 0 0 2	
2.266E+00	7.758E+02	75.1	W013	1 2 1 1 2	
2.290E+00	7.840E+02	79.5	W013	1 2 1 1 2	
1.276E+00	4.366E+02	80	C401	1 0 0 0 0	EFG
1.291E+00	4.417E+02	80	G060	1 0 0 0 2	
1.090E+01	3.730E+03	80	H063	1 0 0 0 2	
2.289E+00	7.835E+02	80	M043	1 0 0 0 2	
2.304E+00	7.886E+02	82.3	W013	1 2 1 1 2	
2.333E+00	7.985E+02	85.1	W013	1 2 1 1 2	
2.335E+00	7.994E+02	85.3	W013	1 2 1 1 2	
2.337E+00	7.999E+02	85.5	W013	1 2 1 1 2	
2.344E+00	8.022E+02	86.6	W013	1 2 1 1 2	
2.346E+00	8.032E+02	88.0	W013	1 2 1 1 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
2.355E+00	8.061E+02	90	G046	1 0 1 1 2	
2.363E+00	8.087E+02	90.2	W013	1 2 1 1 2	
2.388E+00	8.176E+02	95	G046	1 0 1 1 2	
2.409E+00	8.247E+02	98	G046	1 0 1 1 2	
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
2.424E+00	8.296E+02	100	D041	1 0 0 0 2	
2.424E+00	8.296E+02	100	G046	1 0 1 1 2	
2.424E+00	8.296E+02	100	M043	1 0 0 0 2	

2961. $C_{12}H_{23}NO_3$

Propylbutylaceturethane

RN: **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E-03	3.199E-01	20	O021	1 2 0 0 0	

2962. $C_{12}H_{23}N_7$

1-(4′-Methyl-1-piperizinyl)-3,5-bis(dimethylamino)-*s*-triazine

2-(4-Methyl-1-piperazinyl)-4,6-bis(dimethylamino)-*s*-triazine

RN: 5512-05-0 **MP** (°C)**:**

MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.514E-03	1.198E+00	25	B386	0 0 0 0 0	

2963. $C_{12}H_{24}N_2O_2$
N,*N*,*N*′,*N*′-Tetramethylsuberamide
Octanediamide, *N*,*N*,*N*′,*N*′-tetramethyl-
RN: 27397-05-3 **MP** (°C)**:**
MW: 228.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	5.754E+02	30	D010	1 2 1 1 2	

2964. $C_{12}H_{24}N_3O_3PS$
Thiophosphoryl trimorpholide
Morpholine, 4,4′,4″-phosphinothioylidynetris-
Phosphine sulfide, trimorpholino-
RN: 14129-98-7 **MP** (°C)**:**
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.987E-03	3.210E+00	25	A040	1 0 0 0 2	

2965. $C_{12}H_{24}N_3O_4P$
Phosphoryl trimorpholide
Morpholine, 4,4′,4″-phosphinylidynetris-
Phosphine oxide, trimorpholino-
RN: 4441-12-7 **MP** (°C)**:**
MW: 305.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E+00	6.072E+02	25	A040	1 0 0 0 2	

2966. $C_{12}H_{24}N_6$
*N*2,*N*4,*N*6-Triethyl-*N*2,*N*4,*N*6-trimethylmelamine
1,3,5-Triazine-2,4,6-triamine, *N*,*N*′,*N*″-triethyl-*N*,*N*′,*N*″-trimethyl-
RN: 64124-20-5 **MP** (°C)**:**
MW: 252.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-04	5.000E-02	25	C051	1 2 1 1 0	pH 7

2967. $C_{12}H_{24}N_9P_3$
Hexaziridinocyclotriphosphazene
2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis(1-aziridinyl)-1,3,5,2,4,6-triazatriphosphorine
2,2,4,4,6,6-Hexakis(1-aziridinyl)cyclotriphosphaza-1,3,5-triene
Apholate
APN
ENT 26316
RN: 52-46-0 **MP** (°C)**:**
MW: 387.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-01	1.000E+02	ns	L076	0 1 0 0 0	approximate

2968. $C_{12}H_{24}O_2$
Lauric acid
Dodecanoic acid
Laurostearic acid
RN: 143-07-7 **MP** (°C)**:** 44
MW: 200.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.847E-04	3.700E-02	0	B136	1 0 2 1 1	
2.895E-04	5.800E-02	20	B136	1 0 2 1 1	
2.745E-04	5.500E-02	20	D041	1 0 0 0 1	
2.745E-04	5.500E-02	20.0	R001	1 1 1 1 1	
2.400E-05	4.808E-03	25	J001	1 0 2 1 2	
8.486E-06	1.700E-03	25	M083	1 0 0 1 1	
1.150E-05	2.304E-03	25	R002	0 0 0 0 0	intrinsic
2.080E-05	4.167E-03	25	R002	0 0 0 0 0	
3.345E-04	6.700E-02	30	B136	1 0 2 1 1	
3.145E-04	6.300E-02	30.0	R001	1 1 1 1 1	
3.494E-04	7.000E-02	40	B136	1 0 2 1 1	
3.844E-05	7.700E-03	40	E005	2 1 1 2 1	
3.744E-04	7.500E-02	45	B136	1 0 2 1 1	
3.744E-04	7.499E-02	45.0	R001	1 1 1 1 1	
4.593E-05	9.200E-03	50	E005	2 1 1 2 1	
5.470E-05	1.096E-02	50	J001	1 0 2 1 2	
4.343E-04	8.700E-02	60	B136	1 0 2 1 1	
5.791E-05	1.160E-02	60	E005	2 1 1 2 2	
4.343E-04	8.699E-02	60.0	R001	1 1 1 1 1	
1.847E-04	3.700E-02	.0	R001	1 1 1 1 1	

2969. $C_{12}H_{24}O_2$
3-Hydroxy-2,2,5,5-tetraethyltetrahydrofuran
3-Furanol, 2,2,5,5-tetraethyltetrahydro-
RN: 29839-78-9 **MP** (°C)**:**
MW: 200.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.493E-02	2.991E+00	rt	B066	0 2 0 0 0	

2970. $C_{12}H_{24}O_3$
1,3-Dioxolane-4-methanol, 2-heptyl-2-methyl
2-Heptyl-4-hydroxymethyl-2-methyl-1,3-dioxolane
RN: 5660-50-4 **MP** (°C)**:**
MW: 216.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-03	7.701E-01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2971. $C_{12}H_{24}O_4$
1,3-Dioxolane-4-methanol, 2-methyl-2-[2-(pentyloxy)ethyl]
RN: 143458-56-4 **MP** (°C)**:**
MW: 232.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.250E-02	1.452E+01	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

2972. $C_{12}H_{26}$
2-Methylundecane
Isododecane
RN: 31807-55-3 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E-08	2.000E-06	25	T423	0 0 0 0 0	

2973. $C_{12}H_{26}$
3,3,6,6-Tetramethyloctane
RN: 62199-46-6 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-07	2.100E-05	25	T423	0 0 0 0 0	

2974. $C_{12}H_{26}$
Dodecane
N-Dodecane
Alkane C(12)
Duodecane
Bihexyl
Adakane 12
RN: 112-40-3 **MP** (°C)**:** –9.6
MW: 170.34 **BP** (°C)**:** 216.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.931E-08	8.400E-06	22.5	G301	0 0 0 0 0	
2.055E-08	3.500E-06	23	C332	0 0 0 0 0	
1.068E-08	1.820E-06	25	B156	1 0 2 2 2	
4.944E-08	8.422E-06	25	F004	0 0 0 0 0	
5.871E-09	1.000E-06	25	T423	0 0 0 0 0	
3.900E-09	6.643E-07	ns	D348	0 0 0 0 0	
2.231E-08	3.800E-06	ns	H123	0 0 0 0 0	

2975. $C_{12}H_{26}$
2,2,4,6,6-Pentamethylheptane
RN: 13475-82-6 **MP** (°C)**:**
MW: 170.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	2.500E-05	25	T423	0 0 0 0 0	

2976. $C_{12}H_{26}O$
Dodecanol
Dodecyl alcohol
Lauryl alcohol
Undecyl carbinol
RN: 112-53-8 **MP** (°C)**:** 24
MW: 186.34 **BP** (°C)**:** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-06	1.696E-03	16	K011	1 2 1 1 2	
2.300E-05	4.286E-03	25	R002	0 0 0 0 0	
1.560E-05	2.907E-03	34	K011	1 2 1 1 2	
1.930E-05	3.596E-03	49	K011	1 2 1 1 2	

2977. $C_{12}H_{27}N$
Tributylamine
tris-n-Butylamine
N,*N*-Dibutyl-1-butanamine
RN: 102-82-9 **MP** (°C)**:** –70
MW: 185.36 **BP** (°C)**:** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.649E-04	1.418E-01	25.04	V013	2 2 2 2 2	

2978. $C_{12}H_{27}N.4H_2O$
Dodecylamine (tetrahydrate)
RN: 124-22-1 **MP** (°C)**:**
MW: 257.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.776E-03	7.145E-01	ns	R037	0 2 2 1 0	

2979. $C_{12}H_{27}OP$
Tributyl phosphine oxide
Tributylphosphine oxide
TBPO
RN: 814-29-9 **MP** (°C)**:** 64
MW: 218.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E+00	2.260E+02	13.20	H031	1 2 2 2 2	
8.794E-01	1.920E+02	13.40	H031	1 2 2 2 2	
4.718E-01	1.030E+02	16.30	H031	1 2 2 2 2	
1.832E-01	4.000E+01	25	B070	1 2 0 1 1	
2.551E-01	5.570E+01	25.00	H031	1 2 2 2 2	
2.299E-01	5.020E+01	27.00	H032	1 1 2 1 2	
2.244E-01	4.900E+01	27.8	H032	1 1 2 1 2	
2.125E-01	4.640E+01	29.0	H032	1 1 2 1 2	
2.020E-01	4.410E+01	30.2	H032	1 1 2 1 2	
1.974E-01	4.310E+01	31.1	H032	1 1 2 1 2	
1.892E-01	4.130E+01	32.0	H032	1 1 2 1 2	
1.818E-01	3.970E+01	32.5	H032	1 1 2 1 2	
1.626E-01	3.550E+01	34.50	H031	1 2 2 2 2	
1.530E-01	3.340E+01	36.0	H032	1 1 2 1 2	
1.205E-01	2.630E+01	42.6	H032	1 1 2 1 2	
1.063E-01	2.320E+01	46.0	H032	1 1 2 1 2	
1.035E-01	2.260E+01	46.70	H031	1 2 2 2 2	
8.932E-02	1.950E+01	50.4	H032	1 1 2 1 2	
7.466E-02	1.630E+01	56.00	H031	1 2 2 2 2	
5.176E-02	1.130E+01	76.50	H031	1 2 2 2 2	
4.306E-02	9.400E+00	99.00	H031	1 2 2 2 2	

2980. $C_{12}H_{27}O_2P$
Butyl dibutyl phosphinate
Butoxydibutylphosphine oxide
Dibutylbutoxyphosphine oxide
Butyl dibutylphosphinate
RN: 2950-47-2 **MP** (°C)**:**
MW: 234.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	4.500E+00	25	B070	1 2 0 1 1	

2981. $C_{12}H_{27}O_3P$
Diethyl octyl phosphonate
Diethyl octanephosphonate
RN: 1068-07-1 **MP** (°C)**:**
MW: 250.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.99E-04	<2.00E-01	25	B070	1 2 0 1 0	

2982. $C_{12}H_{27}O_3P$
Dibutyl butyl phosphonate
Dibutoxybutylphosphine oxide
Dibutyl butanephosphonate
Dibutyl butylphosphonate
TC 44
RN: 78-46-6 **MP** (°C)**:**
MW: 250.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.000E-01	25	B070	1 2 0 1 0	

2983. $C_{12}H_{27}O_4P$
Tributyl phosphate
Tri-*n*-butyl phosphate
RN: 126-73-8 **MP** (°C)**:**
MW: 266.32 **BP** (°C)**:** 289.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-03	1.075E+00	3.4	H027	2 1 2 2 2	
3.800E-03	1.012E+00	4.0	H027	2 1 2 2 2	
3.593E-03	9.570E-01	5.0	H027	2 1 2 2 2	
2.403E-03	6.400E-01	13.0	H027	2 1 2 2 2	
1.500E-03	3.995E-01	25	B070	1 2 0 1 2	
1.464E-03	3.900E-01	25	B070	1 2 0 1 1	

(*continued*)

2983. $C_{12}H_{27}O_4P$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.253E-02	6.000E+00	25	F300	1 0 0 0 0	
1.585E-03	4.220E-01	25.0	H027	2 1 2 2 2	
1.570E-03	4.180E-01	25.0	H032	2 2 2 1 1	EFG
1.070E-03	2.850E-01	50.0	H027	2 1 2 2 2	
1.239E-03	3.299E-01	ns	F014	0 0 0 0 1	

2984. $C_{12}H_{28}Ge$

Tetrapropylgermanium
Tetra-*n*-propylgermane
RN: 994-65-0 **MP** (°C)**:**
MW: 244.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.320E-08	8.133E-06	25	D346	1 1 2 2 2	

2985. $C_{12}Br_{10}O$

Decabromodiphenyl ether
DBDPO
Decabromodiphenyl oxide
RN: 1163-19-5 **MP** (°C)**:** 298.0
MW: 959.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.606E-08	2.500E-05	25	N326	1 0 0 0 1	average

2986. $C_{12}Cl_8O_2$

Octachlorodibenzo-*p*-dioxin
OCDD
1,2,3,4,6,7,8,9-Octachlorodibenzodioxin
O8CDD
Octachlorodibenzo[b,e][1,4]dioxin
RN: 3268-87-9 **MP** (°C)**:** 330
MW: 459.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-13	4.000E-10	20	F303	1 2 1 2 0	
8.700E-13	4.000E-10	20	W319	1 2 1 2 1	
1.610E-13	7.400E-11	25	S352	2 2 0 2 1	
1.610E-13	7.402E-11	25.0	D330	2 2 1 2 2	
4.350E-12	2.000E-09	40	F303	1 2 1 2 1	
4.350E-12	2.000E-09	40	W319	1 2 1 2 1	
6.750E-13	3.103E-10	40.0	D330	2 2 1 2 2	
3.960E-12	1.821E-09	60.0	D330	2 2 1 2 2	
1.710E-12	7.862E-10	80.0	D330	2 2 1 2 2	
8.374E-13	3.850E-10	ns	W332	0 1 0 2 2	

2987. $C_{12}Cl_{10}$
Decachlorobiphenyl
Decachlorbiphenyl
2,2′,3,3′,4,4′,5,5′,6,6′-Decachlorobiphenyl
RN: 2051-24-3 **MP** (°C)**:** 305
MW: 498.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.211E-11	2.100E-08	22	O311	2 2 1 2 1	
1.300E-12	6.483E-10	25	D331	2 1 2 2 2	
1.303E-11	6.500E-09	25	D335	1 0 0 0 1	
1.490E-11	7.430E-09	25	M342	1 0 1 1 2	
3.209E-11	1.600E-08	25	W025	1 0 2 2 1	
1.300E-12	6.483E-10	25.0	M324	1 2 1 1 2	
1.680E-11	8.378E-09	60	D331	2 1 2 2 2	
1.680E-11	8.378E-09	60.0	M324	1 2 1 1 2	
3.530E-11	1.760E-08	70	D331	2 1 2 2 2	
3.530E-11	1.760E-08	70.0	M324	1 2 1 1 2	
9.930E-11	4.952E-08	80	D331	2 1 2 2 2	
9.930E-11	4.952E-08	80.0	M324	1 2 1 1 2	

2988. $C_{13}H_6Cl_5NO_3$
Oxyclozanide
3,5,6,3′,5′-Pentachloro-2,2′-dihydroxybenzanilide
Zanilox
Diplin
ICI 46638
Zanil
RN: 2277-92-1 **MP** (°C)**:**
MW: 401.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.224E-05	2.900E-02	25	P036	0 0 0 0 0	average of 3, form III
2.665E-06	1.070E-03	25	P036	0 0 0 0 0	average of 3, form II
6.227E-07	2.500E-04	25	P036	0 0 0 0 0	average of 3, form I

2989. $C_{13}H_6Cl_6O_2$
Hexachlorophene
2,2′-Methylenebis[3,4,6-trichlorophenol]
Bilevon
AT-7
Dermadex
Exofene
RN: 70-30-4 **MP** (°C)**:** 164.5
MW: 406.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.142E-04	2.499E-01	22	M048	1 0 1 1 0	EFG
4.669E-05	1.900E-02	25	A008	1 0 0 0 0	EFG
3.441E-04	1.400E-01	25	A010	2 2 2 1 1	0.003N HCl
7.373E-07	3.000E-04	ns	V302	0 0 0 0 0	*sic*

2990. $C_{13}H_7Br_2N_3O_6$
Bromofenoxim
3,5-Dibromo-4-hydroxybenzaldehyde-2,4-dinitrophenyloxime
Faneron
Bromfenim
RN: 13181-17-4 **MP** (°C)**:** 196.5
MW: 461.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.169E-07	1.000E-04	20	M161	1 0 0 0 0	
1.288E-06	5.939E-04	ns	R427	0 0 0 0 0	

2991. $C_{13}H_7F_3N_2O_5$
Fluorodifen
p-Nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether
RN: 15457-05-3 **MP** (°C)**:** 90
MW: 328.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.094E-06	2.000E-03	20	E048	1 2 1 1 0	
6.094E-06	2.000E-03	20	M161	1 0 0 0 0	
<6.09E-06	<2.00E-03	ns	B200	0 0 0 0 0	
6.094E-06	2.000E-03	ns	M061	0 0 0 0 0	

2992. $C_{13}H_8ClFO_2$
4′-Chloro-5-fluoro-2-hydroxy benzophenone
SL 79182
RN: 62433-26-5 **MP** (°C)**:**
MW: 250.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-05	8.999E-03	37	F309	1 0 2 2 2	

2993. $C_{13}H_8ClNO$
CP 31675
2-Chloro-*N*-(2-methyl-6-*t*-butylphenyl)acetamide
RN: 3785-20-4 **MP** (°C)**:** 115
MW: 229.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.306E-03	3.000E-01	ns	M061	0 0 0 0 2	

2994. $C_{13}H_8ClN_3O$
RJ-64
3,4-Pyridyl-(5)-2-chlorophenyl-1,2,4-oxadiazole
RN: 27199-40-2 **MP** (°C)**:**
MW: 257.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.045E-03	1.300E+00	37	C054	2 2 2 1 2	0.1N HCl

2995. $C_{13}H_8Cl_2N_2O_4$
Niclosamide
2′,5-Dichloro-4′-nitrosalicylanilide
2-Chloro-4-nitrophenylamide-6-chlorosalicylic acid
Cestocid
Devermine
Bayluscid
RN: 50-65-7 **MP** (°C)**:** 230
MW: 327.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-05	1.332E-02	25	T426	0 0 0 0 0	
1.987E-05	6.500E-03	rt	M161	0 0 0 0 0	

2996. $C_{13}H_8F_2O_3$
Diflunisal
5-(2,4-Difluorophenyl) salicylic acid
Dolobid
RN: 22494-42-4 **MP** (°C)**:**
MW: 250.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-05	6.186E-03	24.99	K447	0 0 0 0 0	pH 2.0
1.199E-05	3.000E-03	37	Y421	0 0 0 0 0	

2997. $C_{13}H_8N_2O_2$
Phenazine-1-carboxylic acid
PCA
RN: **MP** (°C)**:**
MW: 224.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-04	5.157E-02	5.0	Y409	0 0 0 0 0	
2.300E-04	5.157E-02	10.0	Y409	0 0 0 0 0	
2.400E-04	5.381E-02	15.0	Y409	0 0 0 0 0	
2.500E-04	5.606E-02	20.0	Y409	0 0 0 0 0	

(*continued*)

2997. $C_{13}H_8N_2O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	6.054E-02	25.0	Y409	0 0 0 0 0	
2.900E-04	6.502E-02	30.0	Y409	0 0 0 0 0	
3.200E-04	7.175E-02	35.0	Y409	0 0 0 0 0	
3.500E-04	7.848E-02	40.0	Y409	0 0 0 0 0	
3.900E-04	8.745E-02	45.0	Y409	0 0 0 0 0	
4.400E-04	9.866E-02	50.0	Y409	0 0 0 0 0	
5.100E-04	1.144E-01	55.0	Y409	0 0 0 0 0	

2998. $C_{13}H_8N_2O_2S$

m-Pyridine carboxyphenylisothiocyanate
Picolinic acid, *m*-isothiocyanatophenyl ester
RN: 5174-37-8 **MP** (°C)**:**
MW: 256.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.281E-02	25	K032	2 2 0 1 1	

2999. $C_{13}H_9ClN_2O_4$

4′-Chloro-2-hydroxy-3-nitrobenzanilide
Salicylanilide, 4′-chloro-5-nitro-
Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-5nitro-
RN: 6490-98-8 **MP** (°C)**:** 253–254
MW: 292.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-06	2.210E-03	25	D400	2 0 0 1 2	

3000. $C_{13}H_9ClN_2O_4$

4′-Chloro-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-3-nitro-
Salicylanilide, 4′-chloro-3-nitro-
NSC 22899
4′-Chloro-3-nitrosalicylanilide
RN: 6490-99-9 **MP** (°C)**:**
MW: 292.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.851E-05	8.344E-03	25	D400	2 0 0 1 2	

3001. $C_{13}H_9Cl_2NO_4$
2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether
Chlomethoxyfen
Chlomethoxynil
RN: 32861-85-1 **MP** (°C)**:** 113.5
MW: 314.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.550E-07	3.000E-04	15	M161	1 0 0 0 0	

3002. $C_{13}H_9F_3N_2O_2$
Niflumic acid
2-[3-(Trifluoromethyl)anilino]nicotinic acid
Actol
Flogovital
Donalgin
Landruma
RN: 4394-00-7 **MP** (°C)**:** 204
MW: 282.22 **BP** (°C)**:** 378.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-04	7.714E-02	10	B429	1 0 1 2 2	
2.805E-04	7.917E-02	15	B429	1 0 1 2 2	
2.916E-04	8.231E-02	20	B429	1 0 1 2 2	
3.028E-04	8.544E-02	25	B429	1 0 1 2 2	
3.128E-04	8.827E-02	30	B429	1 0 1 2 2	
3.261E-04	9.203E-02	35	B429	1 0 1 2 2	
6.732E-05	1.900E-02	rt	H302	0 0 2 1 1	intrinsic
1.400E-04	3.950E-02	rt	R431	0 0 0 0 0	Average

3003. $C_{13}H_9N$
Phenanthridine
Phenanthridin
9-Azaphenanthrene
3,4-Benzoisoquinoline
5-Azaphenanthrene
RN: 229-87-8 **MP** (°C)**:** 106.5
MW: 179.22 **BP** (°C)**:** 349

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.674E-03	3.000E-01	20	F300	1 0 0 0 1	

3004. $C_{13}H_9N$
Acridine
2,3,5,6-Dibenzopyridine
Acridin
RN: 260-94-6 **MP** (°C)**:** 107
MW: 179.22 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.735E-02	24	A029	2 0 0 0 1	0.01N KOH
2.142E-04	3.840E-02	24	H106	1 0 2 2 2	
2.143E-04	3.840E-02	24	M303	1 0 1 1 2	
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	EFG
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	

3005. $C_{13}H_9NO$
2-Hydroxyacridine
o-Hydroxyacridine
RN: 22817-17-0 **MP** (°C)**:**
MW: 195.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.904E-03	20	A029	1 0 0 0 0	

3006. $C_{13}H_9NS$
p-Biphenyl isothiocyanate
4-Biphenyl isothiocyanate
RN: 25687-48-3 **MP** (°C)**:**
MW: 211.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	2.958E-03	25	D019	1 1 1 1 1	

3007. $C_{13}H_9NS$
m-Biphenyl isothiocyanate
3-Biphenyl isothiocyanate
RN: 1510-25-4 **MP** (°C)**:**
MW: 211.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	6.339E-03	25	K032	2 2 0 1 1	

3008. $C_{13}H_{10}$
Fluorene
o-Biphenylmethane
2,3-Benzindene
o-Biphenylenemethane
Diphenylenemethane
2,2′-Methylenebiphenyl
RN: 86-73-7 **MP** (°C)**:** 116
MW: 166.22 **BP** (°C)**:** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-06	7.181E-04	6.60	M082	1 1 1 2 2	
4.320E-06	7.181E-04	6.60	M151	2 1 2 2 2	
4.326E-06	7.190E-04	6.64	M183	1 2 1 1 2	
5.820E-06	9.674E-04	13.20	M082	1 1 1 2 2	
5.820E-06	9.674E-04	13.20	M151	2 1 2 2 2	
5.822E-06	9.678E-04	13.24	M183	1 2 1 1 2	
7.240E-06	1.203E-03	18.00	M082	1 1 1 2 2	
7.240E-06	1.203E-03	18.00	M151	2 1 2 2 2	
7.244E-06	1.204E-03	18.04	M183	1 2 1 1 2	
9.012E-06	1.498E-03	20	V416	0 0 0 0 0	
9.720E-06	1.616E-03	24.00	M082	1 1 1 2 2	
9.720E-06	1.616E-03	24.00	M151	2 1 2 2 2	
9.728E-06	1.617E-03	24.04	M183	1 2 1 1 2	
1.137E-05	1.890E-03	24.60	W003	2 2 2 2 2	average of 3
1.179E-05	1.960E-03	25	B319	2 0 1 2 2	
2.790E-05	4.638E-03	25	L301	1 1 2 2 2	
1.143E-05	1.900E-03	25	L332	1 1 1 1 1	
1.191E-05	1.980E-03	25	M064	1 1 2 2 2	
1.014E-05	1.685E-03	25	M071	2 2 2 2 2	
1.190E-05	1.978E-03	25	M342	1 0 1 1 2	
1.010E-05	1.679E-03	25	W300	2 2 2 2 2	
1.014E-05	1.685E-03	25.00	M151	2 1 1 2 2	
1.110E-05	1.845E-03	27.00	M082	1 1 1 2 2	
1.110E-05	1.845E-03	27.00	M151	2 1 2 2 2	
1.111E-05	1.847E-03	27.04	M183	1 2 1 1 2	
1.420E-05	2.360E-03	29.90	W003	2 2 2 2 2	average of 3
1.317E-05	2.190E-03	30.30	W003	2 2 2 2 2	average of 3
1.350E-05	2.244E-03	31.10	M082	1 1 1 2 2	
1.350E-05	2.244E-03	31.10	M151	2 1 2 2 2	
1.353E-05	2.250E-03	31.14	M183	1 2 1 1 2	
2.244E-05	3.730E-03	38.40	W003	2 2 2 2 2	average of 2
2.223E-05	3.695E-03	40	V416	0 0 0 0 0	
2.322E-05	3.860E-03	40.10	W003	2 2 2 2 2	average of 3
3.387E-05	5.630E-03	47.50	W003	2 2 2 2 2	average of 3
3.862E-05	6.420E-03	50.10	W003	2 2 2 2 2	average of 3
3.772E-05	6.270E-03	50.20	W003	2 2 2 2 2	
5.071E-05	8.430E-03	54.70	W003	2 2 2 2 2	average of 3
6.317E-05	1.050E-02	59.20	W003	2 2 2 2 2	
5.298E-05	8.806E-03	60	V416	0 0 0 0 0	
6.678E-05	1.110E-02	60.50	W003	2 2 2 2 2	average of 3

(*continued*)

3008. $C_{13}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.543E-05	1.420E-02	65.10	W003	2 2 2 2 2	average of 3
1.119E-04	1.860E-02	70.70	W003	2 2 2 2 2	average of 3
1.131E-04	1.880E-02	71.90	W003	2 2 2 2 2	
1.293E-04	2.150E-02	73.40	W003	2 2 2 2 2	
1.191E-05	1.980E-03	ns	M344	0 0 0 0 2	

3009. $C_{13}H_{10}BrCl_2O_2PS$

Leptophos
Phenylphosphonothioic acid *O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl ester
Phosvel
NK 711
Velsicol 506
Oleophosvel

RN: 21609-90-5 **MP** (°C)**:** 60
MW: 412.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.280E-09	3.000E-06	10	B324	0 0 0 0 0	
8.707E-09	3.588E-06	10	B324	0 0 0 0 0	
1.699E-07	7.000E-05	20	B169	2 2 1 1 0	
6.095E-08	2.512E-05	20	B300	2 2 1 1 2	
6.095E-08	2.512E-05	20	B324	0 0 0 0 0	
5.096E-08	2.100E-05	20	B324	0 0 0 0 0	
1.141E-08	4.700E-06	20	C053	0 0 0 0 0	
1.213E-08	5.000E-06	22	K137	1 1 2 1 0	
7.280E-08	3.000E-05	24	C105	2 1 2 2 2	
5.824E-06	2.400E-03	25	M161	1 0 0 0 1	*sic*
1.306E-07	5.382E-05	30	B324	0 0 0 0 0	
1.092E-07	4.500E-05	30	B324	0 0 0 0 0	
2.184E-08	9.000E-06	ns	F040	1 2 2 2 0	
1.141E-08	4.700E-06	ns	F071	0 1 2 1 1	
1.699E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG

3010. $C_{13}H_{10}BrCl_2O_3P$

Leptophos oxon
O-(4-Bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphonate
Phosvel oxon

RN: 25006-32-0 **MP** (°C)**:**
MW: 396.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.586E-06	3.400E-03	20.50	B169	2 2 1 1 2	

3011. $C_{13}H_{10}ClNO_2$

4′-Chloro salicylanilide
N-(*p*-Chlorophenyl)-*o*-hydroxybenzamide
N-(*p*-Chlorophenyl)salicylamide
RN: 3679-63-8 **MP** (°C)**:**
MW: 247.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.885E-08	1.210E-05	ns	N336	0 0 0 0 0	intrinsic

3012. $C_{13}H_{10}Cl_2O$

2,4,-Dichloro-6-benzyl-phenol
o-Cresol, 4,6-dichloro-α-phenyl-
2-Benzyl-4,6-dichlorophenol
RN: 19578-81-5 **MP** (°C)**:**
MW: 253.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	5.822E-03	25	B316	0 0 0 0 0	

3013. $C_{13}H_{10}Cl_2O_2$

Dichlorophen
2,2′-Dihydroxy-5,5′-dichlorodiphenylmethane
G-4
RN: 97-23-4 **MP** (°C)**:** 177–178
MW: 269.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-04	3.000E-02	25	M061	1 0 0 0 0	
1.115E-04	3.000E-02	25	M161	1 0 0 0 1	
1.122E-04	3.020E-02	ns	R427	0 0 0 0 0	

3014. $C_{13}H_{10}INO$

Benodanil
2-Iodo-*N*-phenylbenzamide
Iodobenzanilide
Calirus
RN: 15310-01-7 **MP** (°C)**:** 137
MW: 323.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.189E-05	2.000E-02	20	M161	1 0 0 0 1	

3015. $C_{13}H_{10}N_2$
9-Aminoacridine
10-Amino-5-azaanthracene
Monacrin
Izoacridina
Aminacrine
9AA
RN: 90-45-9 **MP** (°C)**:** 241
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 1 0	0.01N KOH

3016. $C_{13}H_{10}N_2$
4-Aminoacridine
4-Acridinamine
RN: 578-07-4 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.360E-02	24	A029	2 0 0 1 0	0.01N KOH

3017. $C_{13}H_{10}N_2$
3-Aminoacridine
3-Acridinamine
RN: 581-29-3 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.914E-02	24	A029	2 0 0 1 1	0.01N KOH

3018. $C_{13}H_{10}N_2$
2-Aminoacridine
2-Acridinamine
RN: 581-28-2 **MP** (°C)**:** 108.5
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	9.712E-03	24	A029	2 0 0 1 0	0.01N KOH

3019. $C_{13}H_{10}N_2$
1-Aminoacridine
1-Acridinamine
RN: 578-06-3 **MP** (°C)**:** 183
MW: 194.24 **BP** (°C)**:** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 0 1	intrinsic

3020. $C_{13}H_{10}N_4O_3$
1-Benzoyloxymethyl allopurinol
4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(benzoyloxy)methyl]-1,5-dihydro-
RN: 98846-65-2 **MP** (°C)**:** 217–219
MW: 270.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.881E-05	2.400E-02	22	B322	0 0 0 0 0	
8.913E-05	2.409E-02	ns	R427	0 0 0 0 0	

3021. $C_{13}H_{10}O$
Benzophenone
α-Oxodiphenylmethane
Diphenylmethanone
Benzoylbenzene
α-Oxoditane
Oxoditane
RN: 119-61-9 **MP** (°C)**:** 48.5
MW: 182.22 **BP** (°C)**:** 305.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.121E-04	7.510E-02	20	H301	0 0 0 0 0	
7.500E-04	1.367E-01	25	F063	1 1 0 0 1	
3.292E-04	6.000E-02	ns	F014	0 0 0 0 0	

3022. $C_{13}H_{10}O_3$
2,4-Dihydroxybenzophenone
RN: 131-56-6 **MP** (°C)**:**
MW: 214.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	7.050E+00	19.99	L452	0 0 0 0 0	
4.255E-02	9.116E+00	24.99	L452	0 0 0 0 0	
4.805E-02	1.029E+01	29.99	L452	0 0 0 0 0	
5.672E-02	1.215E+01	34.99	L452	0 0 0 0 0	
7.396E-02	1.584E+01	39.99	L452	0 0 0 0 0	

(*continued*)

3022. $C_{13}H_{10}O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.659E-02	1.855E+01	44.99	L452	0 0 0 0 0	
1.174E-01	2.515E+01	49.99	L452	0 0 0 0 0	
1.500E-01	3.213E+01	54.99	L452	0 0 0 0 0	
1.925E-01	4.123E+01	59.99	L452	0 0 0 0 0	
2.559E-01	5.482E+01	64.99	L452	0 0 0 0 0	
3.498E-01	7.493E+01	69.99	L452	0 0 0 0 0	

3023. $C_{13}H_{10}O_3$

Phenyl salicylate
Salol
2-Hydroxybenzoic acid phenyl ester

RN: 118-55-8 **MP** (°C)**:** 42.0
MW: 214.22 **BP** (°C)**:** 173.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.002E-04	1.500E-01	25	F300	1 0 0 0 1	
7.469E-05	1.600E-02	ns	B404	0 2 1 1 0	
1.866E-03	3.998E-01	rt	D021	0 0 1 1 0	

3024. $C_{13}H_{10}O_4$

2,3,4-Trihydroxybenzophenone
2,3,4-Trihydroxy-benzophenon

RN: 1143-72-2 **MP** (°C)**:**
MW: 230.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.811E-02	1.108E+01	19.99	L452	0 0 0 0 0	
5.743E-02	1.322E+01	24.99	L452	0 0 0 0 0	
8.057E-02	1.855E+01	29.99	L452	0 0 0 0 0	
1.051E-01	2.420E+01	34.99	L452	0 0 0 0 0	
1.392E-01	3.204E+01	39.99	L452	0 0 0 0 0	
1.831E-01	4.215E+01	44.99	L452	0 0 0 0 0	
2.574E-01	5.927E+01	49.99	L452	0 0 0 0 0	
3.440E-01	7.919E+01	54.99	L452	0 0 0 0 0	
4.723E-01	1.087E+02	59.99	L452	0 0 0 0 0	
6.152E-01	1.416E+02	64.99	L452	0 0 0 0 0	
7.804E-01	1.797E+02	69.99	L452	0 0 0 0 0	

3025. $C_{13}H_{10}O_4$

2,4,6-Trihydroxybenzophenone
2,4,6-Trihydroxy-benzophenon
RN: 3555-86-0 **MP** (°C)**:**
MW: 230.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.347E-02	3.100E+00	22	F300	1 0 0 0 1	

3026. $C_{13}H_{10}O_5$

2,2′,4,4′-Tetrahydroxybenzophenone
RN: **MP** (°C)**:**
MW: 246.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.863E-02	7.050E+00	19.99	L452	0 0 0 0 0	
3.583E-02	8.821E+00	24.99	L452	0 0 0 0 0	
4.538E-02	1.117E+01	29.99	L452	0 0 0 0 0	
6.199E-02	1.526E+01	34.99	L452	0 0 0 0 0	
8.431E-02	2.076E+01	39.99	L452	0 0 0 0 0	
1.079E-01	2.657E+01	44.99	L452	0 0 0 0 0	
1.487E-01	3.661E+01	49.99	L452	0 0 0 0 0	
2.190E-01	5.393E+01	54.99	L452	0 0 0 0 0	
3.285E-01	8.088E+01	59.99	L452	0 0 0 0 0	
4.448E-01	1.095E+02	64.99	L452	0 0 0 0 0	
5.572E-01	1.372E+02	69.99	L452	0 0 0 0 0	

3027. $C_{13}H_{10}O_5$

2,3,4,4′-Tetrahydroxybenzophenone
RN: 31127-54-5 **MP** (°C)**:**
MW: 246.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.578E-02	1.127E+01	19.99	L452	0 0 0 0 0	
6.120E-02	1.507E+01	24.99	L452	0 0 0 0 0	
8.820E-02	2.172E+01	29.99	L452	0 0 0 0 0	
1.202E-01	2.960E+01	34.99	L452	0 0 0 0 0	
1.712E-01	4.215E+01	39.99	L452	0 0 0 0 0	
2.299E-01	5.660E+01	44.99	L452	0 0 0 0 0	
3.216E-01	7.919E+01	49.99	L452	0 0 0 0 0	
4.768E-01	1.174E+02	54.99	L452	0 0 0 0 0	
6.166E-01	1.518E+02	59.99	L452	0 0 0 0 0	
8.432E-01	2.076E+02	64.99	L452	0 0 0 0 0	
1.084E+00	2.669E+02	69.99	L452	0 0 0 0 0	

3028. $C_{13}H_{10}O_6$
Maclurin
2,4,6,3′,4′-Penta-hydroxy-benzophenol
2,4,6,3′,4′-Pentahydroxybenzophenon
RN: 519-34-6 **MP** (°C)**:** 222.5
MW: 262.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-02	5.000E+00	14	F300	1 0 0 0 0	

3029. $C_{13}H_{11}ClF_3N_3O$
San 6706
4-Chloro-5-(dimethylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3(2H)-pyridazinone
RN: 23576-23-0 **MP** (°C)**:** 151
MW: 317.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.305E-05	1.050E-02	23.50	B200	2 0 0 0 2	

3030. $C_{13}H_{11}ClN_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-
RN: 134698-40-1 **MP** (°C)**:**
MW: 274.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-06	1.199E-03	ns	M381	0 1 1 1 2	pH 7.0

3031. $C_{13}H_{11}ClO$
Chlorophene
5-Chloro-2-hydroxydiphenylmethane
Benzylchlorophenol
RN: 120-32-1 **MP** (°C)**:** 48.5
MW: 218.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	4.155E+00	20	A008	1 0 0 0 0	EFG
1.100E-01	2.406E+01	ns	B047	0 0 0 0 0	EFG

3032. $C_{13}H_{11}N$
2-Aminofluorene
9H-Fluoren-2-amine
2-Fluorenamine
RN: 153-78-6 **MP** (°C)**:** 129
MW: 181.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	3.100E-02	rt	N015	0 0 2 2 1	

3033. $C_{13}H_{11}NO_2$
Salicylanilide
2-Hydroxy-*N*-phenylbenzamide
2-Hydroxybenzanilide
RN: 87-17-2 **MP** (°C)**:** 136
MW: 213.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.579E-04	5.500E-02	23	M061	1 0 0 0 1	
2.579E-04	5.500E-02	25	M161	1 0 0 0 1	

3034. $C_{13}H_{11}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,7-dimethyl-
RN: 74103-12-1 **MP** (°C)**:**
MW: 229.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.597E-08	2.200E-05	25	P089	0 0 0 0 0	
1.527E-07	3.500E-05	37	P089	0 0 0 0 0	
2.116E-07	4.850E-05	51	P089	0 0 0 0 0	

3035. $C_{13}H_{11}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,6-dimethyl-
RN: **MP** (°C)**:**
MW: 229.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-07	5.800E-05	25	P089	0 0 0 0 0	
3.054E-07	7.000E-05	37	P089	0 0 0 0 0	
3.817E-07	8.750E-05	51	P089	0 0 0 0 0	

3036. $C_{13}H_{11}NO_5$
Oxolinic acid
5-Ethyl-5,8-dihydro-8-oxo-1,3-dioxolo(4,5-g)quinoline-7-carboxylic acid
Dioxacin
Gramurin
Starner
S-0208
RN: 14698-29-4 **MP** (°C)**:**
MW: 261.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.214E-03	ns	R427	0 0 0 0 0	

3037. $C_{13}H_{11}N_3O_2$
Benquinox
Cerenox
Seredon
Benzoylhydrazone of quinone oxime
RN: 495-73-8 **MP** (°C)**:**
MW: 241.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-05	5.000E-03	ns	M061	0 0 0 0 0	

3038. $C_{13}H_{11}N_3O_2S_2$
2-Sulfanilamidobenzothiazole
RN: **MP** (°C)**:**
MW: 305.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.275E-06	1.000E-03	37	R045	1 2 1 1 1	

3039. $C_{13}H_{11}N_3O_4S_2$
Tenoxicam
Mobiflex
RN: 59804-37-4 **MP** (°C)**:**
MW: 337.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-04	6.190E-02	32	C411	2 1 1 2 1	

3040. $C_{13}H_{11}N_7O_4S$

5-*p*-Nitrobenzenesulfonamidotetrazole

RN: **MP** (°C)**:**
MW: 361.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.214E-05	8.000E-03	37	R045	1 2 1 1 0	

3041. $C_{13}H_{11}O_3P$

4-Carboxyethylphenylphenylphosphinic acid
CPPPA

RN: **MP** (°C)**:**
MW: 246.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.399E-02	3.443E+00	-239.0	W412	0 0 0 0 0	
1.242E-02	3.059E+00	26.7	W412	0 0 0 0 0	
1.676E-02	4.127E+00	45.08	W412	0 0 0 0 0	
1.931E-02	4.754E+00	54.4	W412	0 0 0 0 0	
2.609E-02	6.424E+00	64.15	W412	0 0 0 0 0	
3.477E-02	8.561E+00	75.71	W412	0 0 0 0 0	
4.371E-02	1.076E+01	84.38	W412	0 0 0 0 0	
3.780E+00	9.307E+02	94.52	W412	0 0 0 0 0	

3042. $C_{13}H_{12}$

Diphenylmethane
1,1′-Methylenebis-benzene
Phenylbenzyl
Benzylbenzene

RN: 101-81-5 **MP** (°C)**:** 25.9
MW: 168.24 **BP** (°C)**:** 264.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-05	3.000E-03	24	H116	2 1 0 0 2	
8.381E-05	1.410E-02	25	A001	1 2 2 2 2	
8.381E-05	1.410E-02	25	A017	1 0 0 0 2	
8.710E-05	1.465E-02	25	D001	1 0 0 0 2	

3043. $C_{13}H_{12}$
4-Methylbiphenyl
4-Phenyltoluene
RN: 644-08-6 **MP** (°C)**:** 49.5
MW: 168.24 **BP** (°C)**:** 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-05	1.834E-03	4.9	D330	2 2 1 2 2	
2.410E-05	4.055E-03	25.0	D330	2 2 1 2 2	
4.180E-05	7.032E-03	40.0	D330	2 2 1 2 2	

3044. $C_{13}H_{12}F_2N_6O$
Fluconazole
1H-1,2,4-Triazole-1-ethanol, α(2,4-difluorophenyl)-α-(1H-1,2,4-triazol-1-ylmethyl)
2,4-Difluoro-α,α1-bis(1H-1,2,4-triazol-1-ylmethyl)benzyl alcohol
Diflucan
Triflucan
RN: 86386-73-4 **MP** (°C)**:** 138–140
MW: 306.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.265E-03	1.000E+00	ns	K444	0 0 0 0 0	

3045. $C_{13}H_{12}N_2O$
Carbanilide
Diphenylurea
N,N′-Diphenylurea
RN: 102-07-8 **MP** (°C)**:** 238.0
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-04	1.503E-01	ns	R427	0 0 0 0 0	
7.066E-04	1.500E-01	rt	D021	0 0 1 1 1	

3046. $C_{13}H_{12}N_2O_3$
Phenallymal
5-Allyl-5-phenylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-phenyl-5-(2-propenyl)
Barbituric acid, 5-allyl-5-phenyl
5-Allyl-5-phenylbarbiturate
RN: 115-43-5 **MP** (°C)**:** 156.5
MW: 244.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.499E-03	1.099E+00	20	J030	1 2 2 2 2	
4.272E-03	1.043E+00	25	P350	0 0 0 0 0	intrinsic
7.764E-03	1.896E+00	37	J030	1 2 2 2 2	

3047. $C_{13}H_{12}N_2O_5S$
Nimesulide
N-(4-Nitro-2-phenoxyphenyl)-methanesulfonamide
RN: 51803-78-2 **MP** (°C)**:**
MW: 308.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.400E-02	25	S415	0 0 0 0 0	
7.395E-05	2.280E-02	37	P432	0 0 0 0 0	

3048. $C_{13}H_{12}O$
p-Benzylphenol
4-Benzylphenol
RN: 101-53-1 **MP** (°C)**:** 81.5
MW: 184.24 **BP** (°C)**:** 322

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.427E-04	9.999E-02	25	L021	1 0 0 0 0	

3049. $C_{13}H_{12}O$
o-Benzylphenol
2-Benzylphenol
RN: 28994-41-4 **MP** (°C)**:** 53.5
MW: 184.24 **BP** (°C)**:** 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.085E-03	2.000E-01	25	L021	1 0 0 0 0	

3050. $C_{13}H_{12}O$
Benzhydrol
Diphenylmethanol
RN: 91-01-0 **MP** (°C)**:** 69
MW: 184.24 **BP** (°C)**:** 298

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.714E-03	5.000E-01	20	F300	1 0 0 0 0	
2.800E-03	5.159E-01	25	D007	2 0 1 1 1	

3051. $C_{13}H_{12}O_5$
bis(4-Hydroxy-3-coumarin) acetic acid ethyl ester
RN: 548-00-5 **MP** (°C)**:**
MW: 248.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.188E-04	5.431E-02	ns	R427	0 0 0 0 0	

3052. $C_{13}H_{13}Cl_2N_3O_3$
Glycophen
1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-*N*-(1-methylethyl)-2,4-dioxo-
Iprodial
LFA 2043
Iprodione
RN: 36734-19-7 **MP** (°C)**:** 136
MW: 330.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.937E-05	1.300E-02	20	M161	1 0 0 0 1	

3053. $C_{13}H_{13}NO_2$
α-(β-Naphthyl)-α-alanine
Alanine, 3-(1(4H)-naphthylidene)-
RN: 13913-40-1 **MP** (°C)**:**
MW: 215.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-03	4.865E-01	25	M097	2 2 2 2 2	

3054. $C_{13}H_{13}NO_5$
2-Azetidinecarboxylic acid, 1-[(benzoyloxy)acetyl]-
RN: 115178-74-0 **MP** (°C)**:** 149.5
MW: 263.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.217E-03	1.900E+00	22	N317	1 1 2 1 2	

3055. $C_{13}H_{13}N_3O_3S$

*N*4-Acetyl sulfapyridine
Acetylsulfapyridine
Sulfapyridine acetylee
RN: 19077-98-6 **MP** (°C)**:**
MW: 291.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.098E-03	3.200E-01	37	D084	1 0 1 0 1	
7.207E-04	2.100E-01	37	F075	1 0 2 2 2	
1.119E-03	3.260E-01	37	M057	1 0 0 0 2	pH 5.5

3056. $C_{13}H_{13}N_3O_5S_2$

Succinylsulfathiazole
2-(*N*(4)-Succinylsulfanilamido)thiazole
p-2-Thiazolylsulfamoylsuccinanilic acid
Kaoxidin
Colistatin
Cremosuxidine
RN: 116-43-8 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-03	4.900E-01	38	K006	1 0 0 0 1	

3057. $C_{13}H_{13}O_4P$

Diphenyl methyl phosphate
Methyl diphenyl phosphate
RN: 115-89-9 **MP** (°C)**:**
MW: 264.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.633E-06	9.600E-04	24	H116	2 1 0 0 2	*sic*
7.569E-03	2.000E+00	25	A044	1 0 0 0 0	*sic*

3058. $C_{13}H_{14}$

1,4,5-Trimethylnaphthalene
Naphthalene, 1,4,5-trimethyl-
RN: 2131-41-1 **MP** (°C)**:** 58
MW: 170.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-05	2.100E-03	25	M064	1 1 2 2 1	
1.190E-05	2.026E-03	25	M342	1 0 1 1 2	
1.233E-05	2.100E-03	ns	M344	0 0 0 0 1	

3059. $C_{13}H_{14}F_3N_3O_4$
Ethalfluralin
N-Ethyl-*N*-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine
Buvilan
Solanan
RN: 55283-68-6 **MP** (°C)**:** 55.5
MW: 333.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.001E-07	2.000E-04	25	M161	1 0 0 0 0	pH 7
9.002E-07	3.000E-04	ns	D304	1 0 0 0 0	

3060. $C_{13}H_{14}N_2$
4,4′-Methylenedianiline
4,4′-Methylenebisbenzeneamine
Tonox
HT 972
RN: 101-77-9 **MP** (°C)**:** 93
MW: 198.27 **BP** (°C)**:** 398

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.044E-03	1.000E+00	19	I307	0 0 0 0 0	

3061. $C_{13}H_{14}N_2O_3$
Mephobarbital
5-Ethyl-1-methyl-5-phenylbarbituric acid
5-Ethyl-*N*-methyl-5-phenylbarbituric acid
Mebaral
Prominal
Methylphenobarbital
RN: 115-38-8 **MP** (°C)**:** 176
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-04	1.500E-01	20	J030	1 2 2 2 1	
4.872E-04	1.200E-01	37	J030	1 2 2 2 1	

3062. $C_{13}H_{14}N_2O_6$
Benzoic acid, 2-(acetyloxy)-, 2-[(2-amino-2-oxoethyl)amino]-2-oxoethyl ester
RN: 118247-02-2 **MP** (°C)**:** 186
MW: 294.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-03	8.800E-01	21	N335	0 0 0 0 0	

3063. $C_{13}H_{14}N_4$

Pyridine-2-azo-*p*-dimethylaniline
PADA
2-(*p*-*N*,*N*-Dimethylaminophenylazo)pyridine
p-(2-Pyridylazo)-*N*,*N*-dimethylaniline
N,*N*-Dimethyl-4-(2-pyridylazo)aniline
2-(*p*-*N*,*N*-Dimethylaminophenylazo)pyridine
RN: 13103-75-8 **MP** (°C)**:**
MW: 226.28 **BP** (°C)**:** 392.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-05	2.127E-02	ns	B418	0 2 1 1 2	

3064. $C_{13}H_{14}N_4O_3S$

*N*4-Acetylsulfamerazine
*N*4-Acetylsulphamerazine
2-*N*4-Acetylsulfanilamido-4-methylpyrimidine
RN: 127-73-1 **MP** (°C)**:**
MW: 306.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.676E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
2.579E-03	7.900E-01	37	L091	1 0 0 0 1	pH 5.5
9.140E-04	2.800E-01	37	R045	1 2 1 1 2	
9.140E-04	2.800E-01	37	R045	1 2 1 1 1	
1.234E-03	3.780E-01	37	S192	1 0 1 1 2	pH 6.0
2.611E-03	8.000E-01	38	K006	1 0 0 0 1	

3065. $C_{13}H_{14}N_4O_4S$

Acetyl sulfamethoxypyridazine
3-(*N*1-Acetylsulfanilamido)-6-methoxypyridazine
Acetylmidicel
RN: 127-75-3 **MP** (°C)**:**
MW: 322.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.825E-04	2.200E-01	37	B046	1 0 2 2 1	pH 4.5

3066. $C_{13}H_{14}O_6$

Salicylic acid acetate, hydroxymethyl ester propionate
RN: 32620-70-5 **MP** (°C)**:** 51.5
MW: 266.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.629E-03	7.000E-01	21	N335	0 0 0 0 0	

3067. $C_{13}H_{14}O_6$
Methylphthalyl ethyl glycolate
2-Ethoxy-2-oxoethyl methyl ester
RN: 85-71-2 **MP** (°C)**:** <–35
MW: 266.25 **BP** (°C)**:** 189

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-03	5.297E-01	20	F070	1 0 0 0 2	

3068. $C_{13}H_{15}NO_2$
Glutethimide
Doriden
Noxyron
RN: 77-21-4 **MP** (°C)**:** 84
MW: 217.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.372E-03	9.500E-01	27	B043	1 0 1 2 0	EFG
4.600E-03	9.994E-01	30	D010	1 2 1 1 2	
4.603E-03	1.000E+00	32	B043	1 0 1 2 0	EFG
5.753E-03	1.250E+00	37	B043	1 0 1 2 0	EFG
5.523E-05	1.200E-02	37	B045	1 0 1 1 2	
4.603E-03	1.000E+00	ns	A090	0 0 0 0 1	*sic*
4.600E-03	9.994E-01	ns	R010	0 1 0 0 2	

3069. $C_{13}H_{15}NO_2$
Pyracarbolid
3,4-Dihydro-6-methyl-*N*-phenyl-2H-pyran-5-carboxamide
Sicarol
RN: 24691-76-7 **MP** (°C)**:** 110.5
MW: 217.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.762E-03	6.000E-01	40	M161	1 0 0 0 0	

3070. $C_{13}H_{15}NO_2S$
m-Carboxylpentylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 249.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-05	1.820E-02	25	K032	2 2 0 1 1	

3071. $C_{13}H_{15}NO_3$
Pyrrolidine, 1-[(benzoyloxy)acetyl]-
RN: 115178-67-1 **MP** (°C)**:** 58
MW: 233.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.701E-02	6.300E+00	22	N317	1 1 2 1 2	

3072. $C_{13}H_{15}NO_4$
Morpholine, 4-[(benzoyloxy)acetyl]-
RN: 106231-68-9 **MP** (°C)**:** 103.5
MW: 249.27 **BP** (°C)**:** 453.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-02	4.200E+00	22	B427	1 0 0 1 1	
1.685E-02	4.200E+00	22	N317	1 1 2 1 2	

3073. $C_{13}H_{15}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(dimethylamino)-2-oxoethyl ester
RN: 118247-04-4 **MP** (°C)**:** 75.5
MW: 265.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-02	7.500E+00	21	N335	0 0 0 0 0	

3074. $C_{13}H_{15}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(ethylamino)-2-oxoethyl ester
RN: 118247-01-1 **MP** (°C)**:** 80.5
MW: 265.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-02	5.520E+00	21	N335	0 0 0 0 0	

3075. $C_{13}H_{15}N_3O_2$
Pyrolan
1-Phenyl-3-methylpyrazolyl-5-dimethylcarbamate
RN: 87-47-8 **MP** (°C)**:** 50
MW: 245.28 **BP** (°C)**:** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.138E-03	1.996E+00	ns	M061	0 0 0 0 0	

3076. $C_{13}H_{15}N_3O_3S$
2-Sulfanilamido-3-ethoxypyridine
Benzenesulfonamide, 4-amino-*N*-(3-ethoxy-2-pyridinyl)-
RN: 71119-19-2 **MP** (°C)**:**
MW: 293.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.011E-04	2.350E-01	37	R058	1 2 1 1 2	

3077. $C_{13}H_{15}N_3O_3S$
5-Sulfanilamido-2-ethoxypyridine
Benzenesulfonamide, 4-amino-*N*-(6-ethoxy-3-pyridinyl)-
RN: 71720-65-5 **MP** (°C)**:**
MW: 293.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-04	3.600E-02	37	R058	1 2 1 1 1	

3078. $C_{13}H_{15}N_3O_4S$
Acetyl sulfisoxazole
*N*1-Acetyl-sulfaisoxazole
RN: 80-74-0 **MP** (°C)**:** 193.5
MW: 309.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.586E-04	8.000E-02	37	B046	1 0 2 2 0	pH 4.5
1.199E-04	3.710E-02	37	M117	2 1 1 1 2	pH 6.0

3079. $C_{13}H_{15}N_3O_4S$
*N*1-(3,4-Dimethyl-5-isoxazolyl)-*N*4-acetylsulfanilamide
Acetylsulfadimethylisoxazole
*N*4-Acetylsulfisoxazole
4-*N*-Acetylsulfisoxazole
N-Acetylsulfisoxazole
RN: 4206-74-0 **MP** (°C)**:**
MW: 309.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.450E-02	7.579E+00	37	B110	1 0 2 2 2	pH 6.7

3080. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid 1-ethylpropyl ester
RN: 65267-94-9 **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-05	4.855E-03	ns	M120	0 0 1 1 2	

3081. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-pentyl ester
2,4-D Pentyl ester
Pentyl 2,4-dichlorophenoxyacetate
Amyl 2,4-dichlorophenoxyacetate
RN: 1917-92-6 **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.897E-05	8.436E-03	ns	M120	0 0 1 1 2	

3082. $C_{13}H_{16}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid 2-methylbutyl ester
RN: **MP** (°C)**:**
MW: 291.18 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-05	3.760E-03	ns	M120	0 0 1 1 2	

3083. $C_{13}H_{16}F_3N_3O_4$
Benefin
Benfluralin
RN: 1861-40-1 **MP** (°C)**:** 65
MW: 335.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.98E-06	<1.00E-03	25	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	P028	0 0 0 0 0	
2.088E-04	7.000E-02	ns	M061	0 0 0 0 1	

3084. $C_{13}H_{16}F_3N_3O_4$

Trifluralin
α,α,α-Trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine
RN: 1582-09-8 **MP** (°C)**:** 48.5
MW: 335.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E-05	4.000E-03	20	F311	1 2 2 2 1	
2.419E-05	8.110E-03	22	K137	1 1 2 1 0	
1.730E-06	5.800E-04	25	G319	0 0 0 0 0	
<2.98E-06	<1.00E-03	27	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	P028	0 0 0 0 0	
7.158E-05	2.400E-02	ns	B185	0 0 0 0 0	
1.193E-04	4.000E-02	ns	M061	0 0 0 0 1	
2.088E-06	7.000E-04	ns	M110	0 0 0 0 0	EFG
5.488E-07	1.840E-04	ns	V414	0 0 0 0 0	

3085. $C_{13}H_{16}NO_4PS$

Isoxathion
O,O-Diethyl *O*-5-phenylisoxazol-3-yl phosphorothioate
E-48
Karphos
SI-6711
RN: 18854-01-8 **MP** (°C)**:**
MW: 313.31 **BP** (°C)**:** 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.064E-06	1.900E-03	25	N305	1 0 0 0 1	

3086. $C_{13}H_{16}N_2$

3-(1-Methyl-2-pyrrolidinyl)-indole
RN: **MP** (°C)**:**
MW: 200.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-03	7.030E-01	37	H004	0 0 0 0 0	
3.510E-03	7.030E-01	37	H011	0 0 0 0 0	

3087. $C_{13}H_{16}N_2O_2$

Melatonin
Prime-X
RN: 8041-44-9 **MP** (°C)**:**
MW: 232.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-03	4.344E-01	25	B426	1 1 2 2 2	

3088. $C_{13}H_{16}N_2O_4$
N-Acetyl-L-tyrosinamide acetate
RN: **MP** (°C)**:**
MW: 264.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	3.436E+00	25	A066	1 0 1 1 1	

3089. $C_{13}H_{16}N_2O_4$
Methyl-2-ethyl-2-phenylmalonurate
Methyl 2-ethyl-2-phenylmalonurate
RN: 73632-81-2 **MP** (°C)**:** 105
MW: 264.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.757E-01	23	B152	1 2 1 1 1	pH 3.5

3090. $C_{13}H_{16}N_2O_6$
Medinoterb acetate
m-Cresol, 6-*tert*-butyl-2,4-dinitro-, acetate
MC 1488
RN: 2487-01-6 **MP** (°C)**:** 86.5
MW: 296.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.375E-05	1.000E-02	rt	M161	0 0 0 0 1	

3091. $C_{13}H_{16}N_4O_2S$
2-Sulfanilylamino-4-ethyl-5-methylpyrimidine
RN: **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.551E-04	2.500E-01	37	R076	1 2 0 0 1	

3092. $C_{13}H_{16}N_4O_2S$
2-*p*-Aminobenzenesulphonamido-4,5,6-trimethylpyrimidine
Sulfanilamide, *N*1-(4,5,6-trimethyl-2-pyrimidinyl)-
RN: 5433-64-7 **MP** (°C)**:**
MW: 292.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.131E-04	1.500E-01	37	R075	1 0 0 0 1	

3093. $C_{13}H_{16}N_4O_6.0.5H_2O$

9-[5-*O*-(Acetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
2′-Acetyl-6-methoxypurine arabinoside (hemihydrate)
RN: 121032-43-7 **MP** (°C)**:** 174-176
MW: 333.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-02	1.083E+01	37	C348	0 0 0 0 0	pH 7.00
5.310E-02	1.770E+01	37	M378	1 2 1 1 2	pH 7.2

3094. $C_{13}H_{16}O_4$

Diethylacetyl salicylate
Salicylic acid, 2-ethylbutyrate
RN: 100613-21-6 **MP** (°C)**:**
MW: 236.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.616E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 4.00, intrinsic

3095. $C_{13}H_{16}O_6$

Methyl phthalyl ethyl glycollate
RN: **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.096E-03	1.099E+00	15	H069	1 0 1 1 1	
1.975E-03	5.297E-01	ns	F014	0 0 0 0 1	

3096. $C_{13}H_{16}O_7.0.75H_2O$

Helicin (0.75 hydrate)
Salicylaldehyde β-D-glucoside
Benzaldehyde, 2-(β-D-glucopyranosyloxy)-, hydrate (4:3)
RN: 618-65-5 **MP** (°C)**:**
MW: 297.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.505E-02	1.639E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3097. $C_{13}H_{17}ClO_3$
MCPB-ethyl
RN: 10443-70-6 **MP** (°C)**:**
MW: 256.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.899E-05	1.001E-02	ns	S460	0 0 0 0 0	

3098. $C_{13}H_{17}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-butanoate
5′-Butyryl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-butyrate
RN: 84043-26-5 **MP** (°C)**:** 145.5
MW: 424.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E+03	6.151E+05	25	N332	0 0 0 0 0	pH 7.4

3099. $C_{13}H_{17}IN_2O_6$
Uridine, 2′-deoxy-5-iodo-, 5′-(2-methylpropanoate)
5′-Isobutyryl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-isobutyrate
RN: 84043-27-6 **MP** (°C)**:** 144.5
MW: 424.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E+03	7.423E+05	25	N332	0 0 0 0 0	pH 7.4

3100. $C_{13}H_{17}NO$
N-Butylcinnamamide
N-Butyl-3-phenyl-2-propenamide
RN: 6299-56-5 **MP** (°C)**:**
MW: 203.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	1.972E-01	ns	H350	0 0 0 0 0	

3101. $C_{13}H_{17}NO$
N,N-Diethylcinnamamide
N,N-Diethyl-3-phenyl-2-propenamide
RN: 3680-04-4 **MP** (°C)**:**
MW: 203.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.450E-03	1.514E+00	ns	H350	0 0 0 0 0	

3102. $C_{13}H_{17}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-butyl-
RN: 115193-28-7 **MP** (°C)**:** 69.5
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-03	4.100E-01	22	N317	1 1 2 1 2	

3103. $C_{13}H_{17}NO_3$
N-Acetyl-L-phenylalanine ethyl ester
RN: 2361-96-8 **MP** (°C)**:**
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.550E+00	5	L081	2 1 2 2 2	
1.755E-02	4.130E+00	28	L081	2 1 2 2 2	
2.814E-02	6.620E+00	40	L081	2 1 2 2 2	
3.417E-02	8.040E+00	55	L081	2 1 2 2 2	
7.268E-02	1.710E+01	65	L081	2 1 2 2 2	

3104. $C_{13}H_{17}NO_3$
2-(*p*-Acetaminophenoxy)tetrahydropyran
RN: 51453-65-7 **MP** (°C)**:** 60
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	7.059E-01	ns	H076	0 0 0 0 0	

3105. $C_{13}H_{17}NO_3$
Pivalyl acetaminophen
Propanoic acid, 2,2-dimethyl-, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, pivalate (ester)
RN: 20675-23-4 **MP** (°C)**:** 162.5–163
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.675E-04	1.100E-01	37	D029	0 0 0 0 0	

3106. $C_{13}H_{17}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-(1,1-dimethylethyl)-
RN: 106231-52-1 **MP** (°C)**:** 112–113
MW: 235.29 **BP** (°C)**:** 418.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	B427	1 0 0 1 1	

3107. $C_{13}H_{17}NO_3$

Acetamide, 2-(benzoyloxy)-*N,N*-diethyl-

RN: 64649-63-4 **MP** (°C)**:** 72.5
MW: 235.29 **BP** (°C)**:** 377.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	2.000E+00	22	B427	1 0 0 1 1	in 0.01M HCl
8.500E-03	2.000E+00	22	N317	1 1 2 1 2	

3108. $C_{13}H_{17}NO_3$

Butanamide, 4-(benzoyloxy)-*N,N*-dimethyl-

RN: 115178-78-4 **MP** (°C)**:** 40.5
MW: 235.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.908E-02	1.390E+01	22	N317	1 1 2 1 2	

3109. $C_{13}H_{17}NO_4$

Benzoic acid, 2-hydroxy-, 2-(diethylamino)-2-oxoethyl ester
N,N-Diethylglycolamide salicylate
N,N-Diethyl glycolamide salicylate

RN: 65783-69-9 **MP** (°C)**:** 74–75
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	7.000E-01	21	B331	1 2 2 1 1	pH 7.4
2.786E-03	7.000E-01	21	B331	0 0 0 0 0	

3110. $C_{13}H_{17}NO_4$

Butyl acetaminophen
Carbonic acid, butyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, butyl carbonate (ester)

RN: 19872-68-5 **MP** (°C)**:** 119.5–120
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.367E-04	1.600E-01	37	D029	0 0 0 0 0	

3111. $C_{13}H_{17}NO_4$

Isobutyl acetaminophen
Carbonic acid, isobutyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, isobutyl carbonate (ester)
RN: 20460-96-2 **MP** (°C)**:** 119–121
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.512E-03	3.800E-01	37	D029	0 0 0 0 0	

3112. $C_{13}H_{17}NO_4$

O-(Pivaloyloxymethyl) salicylamide
RN: **MP** (°C)**:** 95
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	1 2 2 1 1	pH 4

3113. $C_{13}H_{17}NO_4$

Propanoic acid, 2,2-dimethyl-, [2-(aminocarbonyl)phenoxy]methyl ester
O-Pivaloyloxymethyl salicylamide
RN: 103951-40-2 **MP** (°C)**:** 94–96
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	0 0 0 0 0	

3114. $C_{13}H_{17}NO_4$

Acetamide, 2-(benzoyloxy)-*N*-ethyl-*N*-(2-hydroxyethyl)-
RN: 106231-60-1 **MP** (°C)**:** 79.5
MW: 251.28 **BP** (°C)**:** 437.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.298E-02	1.080E+01	22	B427	1 0 0 1 1	in 0.01M HCl
4.298E-02	1.080E+01	22	N317	1 1 2 1 2	

3115. $C_{13}H_{17}NO_4$

N-Acetyl-L-tyrosine ethyl ester
Ethyl *N*-acetyl-L-tyrosinate
RN: 840-97-1 **MP** (°C)**:**
MW: 251.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.571E-03	1.400E+00	5	L081	2 1 2 2 2	
1.385E-02	3.480E+00	28	L081	2 1 2 2 2	

3116. $C_{13}H_{17}NO_5$

Acetamide, 2-(benzoyloxy)-*N,N*-bis(2-hydroxyethyl)-

RN: 106231-61-2 **MP** (°C)**:** 81
MW: 267.28 **BP** (°C)**:** 497.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.694E+00	7.200E+02	22	B427	1 0 0 1 1	in 0.01M HCl
2.694E+00	7.200E+02	22	N317	1 1 2 1 2	

3117. $C_{13}H_{17}NO_6$

Acetamide, 2-(benzoyloxy)-*N*-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-

RN: 115193-31-2 **MP** (°C)**:** 126.5
MW: 283.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.401E-02	1.530E+01	22	N317	1 1 2 1 2	

3118. $C_{13}H_{17}N_3O$

Aminopyrine
Amidopyrine
4-Dimethylaminoantipyrine
Febrinina
Febron
Itamidone

RN: 58-15-1 **MP** (°C)**:** 108
MW: 231.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-01	6.540E+01	0	C025	0 0 0 0 2	form A
5.607E-01	1.297E+02	4.62	M109	2 1 1 1 0	EFG
5.463E-01	1.264E+02	10.93	M109	2 1 1 1 0	EFG
5.430E-01	1.256E+02	15.02	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	20	C025	0 0 0 0 2	form A
5.452E-01	1.261E+02	20.96	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	25	P012	0 0 0 0 0	
2.162E-01	5.000E+01	25	P016	1 0 0 1 1	
2.075E-01	4.800E+01	25	P020	2 0 1 1 1	
1.773E+00	4.100E+02	25	P020	2 0 1 1 2	
5.618E-01	1.300E+02	25.35	M109	2 1 1 1 0	EFG
5.965E-01	1.380E+02	29.87	M109	2 1 1 1 0	EFG
2.350E-01	5.436E+01	30	A078	2 1 2 1 0	EFG
2.291E-01	5.300E+01	37	C025	0 0 0 0 2	form A
6.329E-01	1.464E+02	38.37	M109	2 1 1 1 0	EFG
6.646E-01	1.537E+02	49.42	M109	2 1 1 1 0	EFG
3.415E-01	7.900E+01	55	C025	0 0 0 0 2	form A
5.638E-01	1.304E+02	65	C025	0 0 0 0 2	form A
2.162E+00	5.000E+02	69.50	C025	0 0 0 0 2	form A

(*continued*)

3118. $C_{13}H_{17}N_3O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E+00	4.000E+02	70	C025	0 0 0 0 2	form B
1.167E+00	2.700E+02	70.50	C025	0 0 0 0 2	form B
2.879E+00	6.660E+02	74.40	C025	0 0 0 0 2	form B
8.647E-01	2.000E+02	77.50	C025	0 0 0 0 2	form B
6.485E-01	1.500E+02	81	C025	0 0 0 0 2	form B
3.243E+00	7.500E+02	84	C025	0 0 0 0 2	form B
3.359E+00	7.770E+02	92	C025	0 0 0 0 2	form B

3119. $C_{13}H_{17}N_5O_5$

9-(2-*O*-Propionyl-β-D-arabinofuranosyl)adenine

RN: 65174-99-4 **MP** (°C)**:**
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-04	1.170E-01	37	B306	1 2 0 1 2	pH 7.3

3120. $C_{13}H_{17}N_5O_5$

9-[5′-(*O*-Propionyl)-β-D-arabinofuranosyl]adenine ester

RN: 14000-32-9 **MP** (°C)**:** 202.0
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-02	9.200E+00	ns	B134	0 1 1 1 1	

3121. $C_{13}H_{17}N_5O_6$

9-(1,3-Diacetate-2-propoxymethyl)guanine

RN: 86357-19-9 **MP** (°C)**:** 238
MW: 339.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-03	5.800E-01	25	B360	0 0 0 0 0	

3122. $C_{13}H_{17}N_5O_8$

9-(1,3-Dimethoxycarbonyl-2-propoxymethyl)guanine

RN: 91625-66-0 **MP** (°C)**:** 178
MW: 371.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E-04	1.430E-01	25	B360	0 0 0 0 0	

3123. $C_{13}H_{18}ClNO$

Monalide
N-(4-Chlorophenyl)-2,2-dimethylvaleramide
RN: 7287-36-7 **MP** (°C)**:** 87.5
MW: 239.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.510E-05	2.280E-02	23	M161	1 0 0 0 2	
9.510E-05	2.280E-02	ns	M061	0 0 0 0 2	

3124. $C_{13}H_{18}ClNO$

Pentanochlor
Solan
Pentamide, *N*-(3-chloro-4-methylphenyl)-2-methyl-
RN: 2307-68-8 **MP** (°C)**:** 84
MW: 239.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.337E-05	8.000E-03	ns	B185	0 0 0 0 0	
3.545E-05	8.500E-03	rt	M161	0 0 0 0 0	

3125. $C_{13}H_{18}ClN_3O_4S_2$

Cyclopenthiazide
6-Chloro-3-cyclopentylmethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulphonamide 1,1-dioxide
RN: 742-20-1 **MP** (°C)**:** 235
MW: 379.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-04	5.000E-02	rt	A095	0 0 2 2 0	

3126. $C_{13}H_{18}Cl_2N_2O_2$

Melphalan
4-[bis(2-Chloroethyl)amino]-L-phenylalanine
RN: 148-82-3 **MP** (°C)**:**
MW: 305.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	4.400E+00	30	L343	2 1 1 1 0	EFG
5.561E-03	1.697E+00	ns	S469	0 0 0 0 0	

3127. $C_{13}H_{18}N_2O_2$

Lenacil
3-Cyclohexyl-5,6-trimethyleneuracil
RN: 2164-08-1 **MP** (°C)**:** 290
MW: 234.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-05	6.000E-03	25	M061	1 0 0 0 0	
2.561E-05	6.000E-03	25	M161	1 0 0 0 0	

3128. $C_{13}H_{18}N_2O_3$

Heptabarbital
5-(1-Cyclohepten-1-yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-(1-Cyclohepten-1-yl)-5-ethylbarbituric acid
Heptabarbitone
RN: 509-86-4 **MP** (°C)**:** 174
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.503E-01	25	V033	2 0 1 1 2	
1.000E-03	2.503E-01	25.00	T303	1 0 0 0 1	
1.400E-03	3.504E-01	35.00	T303	1 0 0 0 1	
1.170E-02	2.929E+00	40	N008	1 0 1 1 2	*sic*
1.800E-03	4.505E-01	45.00	T303	1 0 0 0 1	

3129. $C_{13}H_{18}N_2O_3S$

Tosylcyclopentylurea
Tosylcyclopentyluree
RN: 1027-87-8 **MP** (°C)**:**
MW: 282.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.649E-04	7.478E-02	37	A028	1 0 2 1 2	intrinsic
2.650E-04	7.483E-02	37	A046	2 0 1 1 2	

3130. $C_{13}H_{18}N_2O_4$

Methyl-2-methyl-2-cyclohexenyl-6-methylmalonurate
Methyl 2-methyl-2-cyclohexenyl-6-methylmalonurate
RN: **MP** (°C)**:** 94
MW: 266.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.592E-01	23	B152	1 2 1 1 1	pH 3.5

3131. $C_{13}H_{18}N_4O_2S_2$

4-Amino-*N*-(5-pentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Benzenesulfonamide, 4-amino-*N*-(5-pentyl-1,3,4-thiadiazol-2-yl)-
RN: 71119-30-7 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	3.656E-02	37	A046	2 0 1 1 2	

3132. $C_{13}H_{18}N_4O_2S_2$

4-Amino-*N*-(5-isopentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Benzenesulfonamide, 4-amino-*N*-[5-(3-methylbutyl)-1,3,4-thiadiazol-2-yl]-
RN: 71119-29-4 **MP** (°C)**:**
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.938E-02	37	A046	2 0 1 1 2	

3133. $C_{13}H_{18}O_2$

Ibuprofen
2-(4-Isobutylphenyl)propionic acid
Advil
Ebufac
Rufen
RS-Ibuprofen
RN: 15687-27-1 **MP** (°C)**:** 75
MW: 206.29 **BP** (°C)**:** 319.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
3.340E-05	6.890E-03	5	F306	1 0 1 2 2	intrinsic
1.080E-04	2.228E-02	12	B411	1 1 1 2 2	
1.460E-04	3.012E-02	20	B411	1 1 1 2 2	
7.271E-05	1.500E-02	20	N316	1 0 1 1 0	EFG
3.102E-04	6.400E-02	21	B331	1 2 2 1 2	pH 7.4
2.375E-04	4.900E-02	25	A408	2 0 1 2 0	int
1.018E-04	2.100E-02	25	A427	0 0 0 0 0	
5.478E-05	1.130E-02	25	C314	0 0 0 0 0	
5.560E-05	1.147E-02	25	C314	0 0 0 0 0	
9.430E-04	1.945E-01	25	D345	0 0 0 0 0	
4.300E-05	8.870E-03	25	F301	1 1 0 0 1	pH 2.0, *sic*
4.300E-05	8.870E-03	25	F306	1 0 1 2 2	intrinsic
5.520E-05	1.139E-02	25	G431	0 0 0 0 0	
2.424E-04	5.000E-02	25	S450	0 0 0 0 0	Intrinsic
2.090E-04	4.311E-02	29	B411	1 1 1 2 2	
7.505E-05	1.548E-02	30	G431	0 0 0 0 0	
1.212E-04	2.500E-02	30	N316	1 0 1 1 0	EFG

(*continued*)

3133. $C_{13}H_{18}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.970E-05	2.057E-02	35	G431	0 0 0 0 0	
5.210E-05	1.075E-02	37	F306	1 0 1 2 2	intrinsic
1.551E-04	3.200E-02	37	N316	1 0 1 1 0	EFG
5.332E-05	1.100E-02	37	P432	0 0 0 0 0	
2.909E-04	6.000E-02	37	Y421	0 0 0 0 0	
3.040E-04	6.271E-02	38	B411	1 1 1 2 2	
1.281E-04	2.643E-02	40	G431	0 0 0 0 0	
4.760E-04	9.819E-02	47	B411	1 1 1 2 2	
1.600E-04	3.301E-02	50	M335	1 0 2 1 2	pH 5
2.036E-04	4.200E-02	50	N316	1 0 1 1 0	EFG
2.327E-04	4.800E-02	60	N316	1 0 1 1 0	EFG
2.600E-04	5.363E-02	ns	F327	0 0 1 2 2	
4.848E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.018E-04	2.100E-02	rt	H302	0 0 2 1 2	intrinsic
4.096E-04	8.450E-02	rt	R431	0 0 0 0 0	Average

3134. $C_{13}H_{18}O_2$

S-Ibuprofen
(*S*)-(+)-2-(4-Isobutylphenyl)propionic acid
D-Ibuprofen
Seractil
Dexibuprofen

RN: 51146-56-6 **MP** (°C)**:**
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
2.560E-04	5.281E-02	12	B411	1 1 1 2 2	
3.390E-04	6.993E-02	20	B411	1 1 1 2 2	
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	
4.670E-04	9.634E-02	29	B411	1 1 1 2 2	
6.090E-04	1.256E-01	38	B411	1 1 1 2 2	

3135. $C_{13}H_{18}O_2$

r-Ibuprofen
(*R*)-2-(4-Isobutylphenyl)propanoic acid
r-(–)-*p*-Isobutylhydratropic acid
l-Ibuprofen

RN: 51146-57-7 **MP** (°C)**:**
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	

3136. $C_{13}H_{18}O_3$

Hexyl *p*-hydroxybenzoate
4-Hydroxybenzoic acid *N*-hexyl ester
RN: 1083-27-8 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.680E-04	8.180E-02	15	B355	0 0 0 0 0	
3.810E-04	8.469E-02	20	B355	0 0 0 0 0	
6.190E-04	1.376E-01	25	B355	0 0 0 0 0	
1.704E-03	3.789E-01	25	D081	1 2 2 1 2	
3.162E-04	7.029E-02	25	F322	2 0 1 1 0	EFG

3137. $C_{13}H_{18}O_3$

n-Hexyl salicylate
n-Hexyl 2-hydroxybenzoate
RN: 6259-76-3 **MP** (°C)**:**
MW: 222.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-03	2.800E-01	37	D009	1 2 1 1 1	0.1N HCl

3138. $C_{13}H_{18}O_5S$

Ethofumesate
2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate
Nortran
Tramat
RN: 26225-79-6 **MP** (°C)**:** 71
MW: 286.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	5.034E-02	25	H434	0 0 0 0 0	
3.841E-04	1.100E-01	25	M161	1 0 0 0 2	
3.841E-04	1.100E-01	25	W313	1 0 0 0 1	

3139. $C_{13}H_{18}O_7$

Salicin
2-(Hydroxymethyl)phenyl-β-D-glucopyranoside
Salicoside
RN: 138-52-3 **MP** (°C)**:** 199
MW: 286.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	4.000E+01	25	F300	1 0 0 0 0	
9.082E-01	2.600E+02	100	F300	1 0 0 0 1	
1.455E-01	4.167E+01	c	D004	0 0 0 0 0	
8.733E-01	2.500E+02	h	D004	0 0 0 0 0	

3140. $C_{13}H_{19}NO_2$
Hexyl *p*-aminobenzoate
4-Aminobenzoic acid hexyl ester
RN: 55791-76-9 **MP** (°C)**:**
MW: 221.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.302E-02	37	F006	1 1 2 2 2	
4.500E-05	9.959E-03	ns	M066	0 0 0 0 1	
4.300E-05	9.516E-03	rt	B016	0 0 1 1 1	pH 7.4

3141. $C_{13}H_{19}NO_2$
Ibuproxam
2-(4-Isobutylphenyl)propionohydroxamic acid
Ibudros
RN: 53648-05-8 **MP** (°C)**:** 123
MW: 221.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.037E-04	2.000E-01	ns	M148	0 2 0 0 0	

3142. $C_{13}H_{19}NO_4$
N,N-Diethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone
RN: **MP** (°C)**:**
MW: 253.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-01	2.920E+01	20	K050	1 1 1 1 2	

3143. $C_{13}H_{19}NO_4S$
Probenecid
Parabenem
4-((Dipropylamino)sulfonyl)benzoic acid
p-(Dipropylsulfamoyl)benzoic
RN: 57-66-9 **MP** (°C)**:** 195
MW: 285.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E-05	3.600E-03	22.5	B422	2 0 2 2 2	
2.089E-06	5.962E-04	ns	R427	0 0 0 0 0	

3144. $C_{13}H_{19}N_3O_4$

N-(1-Ethylpropyl)-2,6-dinitro-3,4-xylidine
Pendimethalin
RN: 40487-42-1 **MP** (°C)**:** 56.5
MW: 281.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-06	3.000E-04	20	M161	1 0 0 0 0	
1.081E-03	3.040E-01	ns	B185	0 0 0 0 0	
1.066E-06	3.000E-04	ns	V414	0 0 0 0 0	

3145. $C_{13}H_{19}N_3O_6S$

Nitralin
4-(Methylsulfonyl)-2,6-dinitro-*N,N*-dipropylaniline
RN: 4726-14-1 **MP** (°C)**:** 151
MW: 345.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-06	6.000E-04	22	M161	1 0 0 0 0	
1.737E-06	6.000E-04	25	B200	1 0 0 0 0	
1.737E-07	6.000E-05	25	P028	0 0 0 0 0	
1.737E-06	6.000E-04	ns	M061	0 0 0 0 0	

3146. $C_{13}H_{20}N_2O$

Prilocaine
RN: 721-50-6 **MP** (°C)**:**
MW: 220.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	6.169E+00	25	D402	1 2 2 2 0	EFG
2.900E-02	6.389E+00	37	D402	1 2 2 2 0	EFG

3147. $C_{13}H_{20}N_2O_2$

Procaine
Novacaine
Novokain
RN: 59-46-1 **MP** (°C)**:** 60
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	9.453E+00	30	L068	1 0 0 1 0	EFG
4.200E-02	9.925E+00	37.5	L034	2 2 0 1 2	pH 7.4
5.494E-03	1.298E+00	ns	E031	0 0 2 1 2	
2.700E-02	6.381E+00	ns	M066	0 0 0 0 1	

3148. $C_{13}H_{20}N_2O_2$
N,N′-Diethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide
RN: **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.216E-02	7.600E+00	20	K050	1 1 1 1 2	

3149. $C_{13}H_{20}N_2O_2$
4-Aminobenzoic acid-2-(butyl-amino)ethyl ester
2-(Butylamino)ethyl 4-aminobenzoate
RN: **MP** (°C)**:**
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	4.017E-02	ns	M066	0 0 0 0 1	

3150. $C_{13}H_{20}N_2O_3$
5-Allyl-5-ethylbutylbarbituric acid
RN: **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.587E-02	4.004E+00	20	J030	1 2 2 2 2	
2.579E-02	6.507E+00	37	J030	1 2 2 2 2	

3151. $C_{13}H_{20}N_2O_3$
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1,1-dimethylethyl)-5-(3-methyl-2-butenyl)
5-*t*-Butyl-5-(3-methylbut-2-enyl)barbiturate
RN: 143585-02-8 **MP** (°C)**:**
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-04	7.090E-02	25	P350	0 0 0 0 0	intrinsic

3152. $C_{13}H_{20}O$
2-Hexyl-6-methylphenol
o-Cresol, 6-hexyl-
RN: 106593-25-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3153. $C_{13}H_{20}O$

2-Hexyl-4-methylphenol
2-Hexyl-*p*-cresol
RN: 54612-53-2 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	6.667E-03	25	L020	1 0 0 0 0	

3154. $C_{13}H_{20}O$

b-Damascone
b-Damascone, *trans*-
trans-2,6,6-Trimethyl-1-crotonylcyclohex-1-ene
trans-*b*-Damascone
Damascone β
RN: 23726-91-2 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	25	D407	1 0 2 2 2	

3155. $C_{13}H_{20}O$

β-Damascone
4-(2,6,6-Trimethyl cyclohex-1-enyl)but-2-en-4-one
Damasione
RN: 23726-92-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	ns	S460	0 0 0 0 0	

3156. $C_{13}H_{20}O$

o-*n*-Heptylphenol
2-*n*-Heptylphenol
RN: 5284-22-0 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.118E-05	1.176E-02	25	L022	1 0 0 0 0	

3157. $C_{13}H_{20}O$
4-Hexyl-2-methylphenol
o-Cresol, 4-hexyl-
RN: 3280-61-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3158. $C_{13}H_{20}O$
α-Ionone
α-Irisone
Cyclocitrylideneacetone
Ionone α
Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
RN: 127-41-3 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-04	1.059E-01	ns	S460	0 0 0 0 0	

3159. $C_{13}H_{20}O$
p-*n*-Heptylphenol
4-*n*-Heptylphenol
RN: 1987-50-4 **MP** (°C)**:**
MW: 192.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.778E-05	1.111E-02	25	L022	1 0 0 0 0	

3160. $C_{13}H_{21}NO_3$
Salbutamol
Albuterol
Ventolin
RN: 18559-94-9 **MP** (°C)**:** 151
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.771E+01	20	M380	1 0 2 1 0	EFG
7.500E-02	1.795E+01	25	M380	1 0 2 1 0	EFG
7.400E-02	1.771E+01	37	M380	1 0 2 1 0	EFG
5.885E-02	1.408E+01	ns	A092	0 0 0 0 0	

3161. $C_{13}H_{21}O_3PS$

S-Benzyl *O,O*-di-isopropyl phosphorothioate
Isokitazine
Kitazin P
IBP
Iprobenfos
Kitazin L

RN: 26087-47-8 **MP** (°C)**:**
MW: 288.35 **BP** (°C)**:** 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-03	1.000E+00	18	M161	1 0 0 0 0	

3162. $C_{13}H_{21}O_4PS$

4-(Methylthio)phenyl dipropyl phosphate
O,O-Dipropyl *O*-4-methylthiophenyl phosphate
Propaphos
Kayaphos
Kayphosnac

RN: 7292-16-2 **MP** (°C)**:**
MW: 304.35 **BP** (°C)**:** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.107E-04	1.250E-01	25	M161	1 0 0 0 2	

3163. $C_{13}H_{22}NO_3PS$

Fenamiphos
1-(Methylethyl)-*O*-ethyl-*O*-(3-methyl-4-(methylthio)phenyl)phosphoramidate
Nemacur
Bay 68138

RN: 22224-92-6 **MP** (°C)**:**
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-03	3.059E-01	10	B324	0 0 0 0 0	
1.009E-03	3.061E-01	10	B324	0 0 0 0 0	
2.291E-03	6.950E-01	20	B179	0 0 0 0 0	
1.084E-03	3.288E-01	20	B300	2 1 1 1 2	
1.085E-03	3.291E-01	20	B324	0 0 0 0 0	
1.084E-03	3.289E-01	20	B324	0 0 0 0 0	
1.381E-03	4.189E-01	30	B324	0 0 0 0 0	
1.381E-03	4.188E-01	30	B324	0 0 0 0 0	
2.307E-03	7.000E-01	rt	M161	0 0 0 0 2	

3164. $C_{13}H_{22}N_2O$
Isonoruron
Urea, 3-[hexahydro-4,7-methanoindan-1(or 2)-yl]-1,1-dimethyl-
Tricuron
BAS 2103H
RN: 28346-65-8 **MP** (°C)**:** 165
MW: 222.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.895E-04	2.200E-01	20	M161	1 0 0 0 2	

3165. $C_{13}H_{22}N_2O$
Noruron
3-(Hexahydro-4,7-methanoindan-5-yl)-1,1-dimethylurea
Norea
RN: 18530-56-8 **MP** (°C)**:** 171
MW: 222.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-04	1.500E-01	20	M061	1 0 0 0 2	
6.747E-04	1.500E-01	25	B200	1 0 0 0 2	
6.747E-04	1.500E-01	ns	G036	0 0 0 0 2	

3166. $C_{13}H_{22}N_2O_3$
5-Ethyl-5-*n*-heptylbarbituric acid
5-Ethyl-5-heptylbarbituric acid
5-Ethyl-5-heptylbarbiturate
RN: 60784-70-5 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.050E-04	1.539E-01	25	M310	2 2 2 2 2	

3167. $C_{13}H_{22}O_3$
Methyl dihydrojasmonate
Hedione
Methyl 3-oxo-2-pentylcyclopentaneacetate
Claigeon
RN: 24851-98-7 **MP** (°C)**:**
MW: 226.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.767E-03	3.998E-01	25	M350	1 0 1 1 1	

3168. $C_{13}H_{24}N_3O_3PS$

Pirimiphos-ethyl
Diethyl *O*-(2-(diethylamino)-6-methyl-4-pyrimidinyl) phosphorothioate
Fernex
Primotec
Solgard
RN: 23505-41-1 **MP** (°C)**:**
MW: 333.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-05	3.967E-03	20	B300	2 1 1 1 2	
<3.00E-06	<1.00E-03	30	M161	1 0 0 0 0	

3169. $C_{13}H_{24}N_4O_3S$

Bupirimate
5-Butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate
Nimrod
RN: 41483-43-6 **MP** (°C)**:** 50.5
MW: 316.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.918E-05	2.189E-02	ns	R427	0 0 0 0 0	
6.953E-05	2.200E-02	rt	M161	0 0 0 0 1	

3170. $C_{13}H_{24}N_6$

1-(Hexamethyleneiminel)-3,5-bis(dimethylamino)-*s*-triazine
1,3,5-Triazine-2,4-diamine, 6-(hexahydro-1H-azepin-1-yl)-*N,N,N′,N′*-tetramethyl-
RN: 125867-92-7 **MP** (°C)**:**
MW: 264.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-05	5.988E-03	25	B386	0 0 0 0 0	

3171. $C_{13}H_{24}O_4$

Octyl α-acetoxypropionate
Propanoic acid, 2-(acetyloxy)-, octyl ester
RN: 6283-90-5 **MP** (°C)**:**
MW: 244.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.093E-04	1.000E-01	25	R006	2 2 0 1 1	

3172. $C_{13}H_{24}O_4$

1,11-Undecanedicarboxylic acid
1,13-Tridecanedioic acid
Brassylic acid
RN: 505-52-2 **MP** (°C)**:** 111
MW: 244.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.139E-03	1.500E+00	21	B040	1 0 1 1 1	*sic*
1.637E-04	4.000E-02	24	F300	1 0 0 0 0	*sic*

3173. $C_{13}H_{25}NO_3$

Dibutylaceturethane
RN: **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.287E-04	7.999E-02	44	O021	1 2 0 0 0	

3174. $C_{13}H_{26}N_2O_2$

N,N,N′,N′-Tetramethylazelamide
Nonanediamide, *N,N,N′,N′*-tetramethyl-
RN: 13424-87-8 **MP** (°C)**:**
MW: 242.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E+00	9.452E+02	30	D010	1 2 1 1 2	

3175. $C_{13}H_{26}O_2$

n-Tridecanoic acid
Tridecanoic acid
RN: 638-53-9 **MP** (°C)**:** 41.5
MW: 214.35 **BP** (°C)**:** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.797E-05	2.100E-02	0	B136	1 0 2 1 1	
1.540E-04	3.300E-02	20	B136	1 0 2 1 1	
1.539E-04	3.300E-02	20.0	R001	1 1 1 1 1	
1.773E-04	3.800E-02	30	B136	1 0 2 1 1	
1.773E-04	3.800E-02	30.0	R001	1 1 1 1 1	
2.053E-04	4.400E-02	45	B136	1 0 2 1 1	
2.053E-04	4.400E-02	45.0	R001	1 1 1 1 1	
2.519E-04	5.400E-02	60	B136	1 0 2 1 1	
2.519E-04	5.400E-02	60.0	R001	1 1 1 1 1	
9.797E-05	2.100E-02	.0	R001	1 1 1 1 1	

3176. $C_{13}H_{26}O_2$
Methyl laurate
Dodecanoic acid methyl ester
Methyl dodecanoate
RN: 111-82-0 **MP** (°C)**:** 41
MW: 214.35 **BP** (°C)**:** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.05E-05	<4.40E-03	20	M337	2 1 2 2 1	

3177. $C_{13}H_{26}O_3$
n-Octyl β-ethoxypropionate
RN: **MP** (°C)**:**
MW: 230.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.34E-04	<10.00E-02	25	D002	1 2 1 1 0	

3178. $C_{13}H_{26}O_3$
Decyl lactate
2-Hydroxypropionic acid decyl ester
RN: 42175-34-8 **MP** (°C)**:**
MW: 230.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.682E-04	2.000E-01	25	R006	2 2 0 1 0	

3179. $C_{13}H_{26}O_4$
1,3-Dioxolane-4-methanol, 2-[2-(hexyloxy)ethyl]-2-methyl
RN: 124485-63-8 **MP** (°C)**:**
MW: 246.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	3.942E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

3180. $C_{13}H_{28}$
Tridecane
RN: 629-50-5 **MP** (°C)**:** –5.5
MW: 184.37 **BP** (°C)**:** 235.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.170E-09	4.000E-07	25	T423	0 0 0 0 0	

3181. $C_{14}H_4N_2O_2S_2$

Dithianon
1,4-Dithiaanthraquinone-2,3-dinitrile
2,3-Dicyano-1,4-dithiaantraquinone
RN: 3347-22-6 **MP** (°C)**:** 225
MW: 296.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-06	5.000E-04	ns	A305	0 0 0 0 0	
4.677E-07	1.386E-04	ns	R427	0 0 0 0 0	

3182. $C_{14}H_6Cl_2F_4N_2O_2$

Teflubenzuron
Nomolt
RN: 83121-18-0 **MP** (°C)**:**
MW: 381.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.466E-08	9.400E-06	20	M402	0 0 0 0 0	

3183. $C_{14}H_6N_2O_4$

1,4,5,8-Naphthalenediimide
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide
1,4,5,8-Naphthalenetetracarboxylic acid diimide
1,4,5,8-Naphthalenetetracarboxylic diimide
Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone
RN: 5690-24-4 **MP** (°C)**:**
MW: 266.21 **BP** (°C)**:** 656.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		23	B410	2 1 2 2 2	

3184. $C_{14}H_6O_8$

Ellagic acid
2,3,7,8-Tetrahydroxy(1)benzopyrano(5,4,3-cde)(1)benzopyran-5,10-dione
Elagostasine
Benzoaric acid
Alizarine yellow
4,4′,5,5′,6,6′-Hexahydrodiphenic acid 2,6,2′,6′-dilactone
RN: 476-66-4 **MP** (°C)**:** >360
MW: 302.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.210E-05	9.700E-03	37	B438	0 0 0 0 0	

3185. $C_{14}H_7ClO_5S$

1,5-Chloroanthraquinone sulfonic acid
1-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-
RN: **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.033E+00	3.333E+02	18	F047	1 2 1 1 0	

3186. $C_{14}H_7ClO_5S$

1,7-Chloroanthraquinone sulfonic acid
RN: **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3187. $C_{14}H_7ClO_5S$

1,6-Chloroanthraquinone sulfonic acid
2-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-
RN: 300360-23-0 **MP** (°C)**:**
MW: 322.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3188. $C_{14}H_8Cl_2N_4$

Clofentezine
3,6-bis(2-Chlorophenyl)-1,2,4,5-tetrazine
Apollo
Acaristop
bis(2-Chlorophenyl)-1,2,4,5-tetrazine
Panatac
RN: 74115-24-5 **MP** (°C)**:** 182.3
MW: 303.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-09	2.522E-06	ns	R424	0 0 0 0 0	
8.318E-09	2.522E-06	ns	R427	0 0 0 0 0	

3189. $C_{14}H_8Cl_4$

2,4′-Dichlorodiphenyldichloroethylene
1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethylene
o,p′-DDE
RN: 3424-82-6 **MP** (°C)**:** 76.5
MW: 318.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.402E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 µm

3190. $C_{14}H_8Cl_4$

p,p′-Dichlorodiphenyldichloroethylene
2,2-bis(4-Chlorophenyl)-1,1-dichloroethylene
p,p′-DDE
RN: 72-55-9 **MP** (°C)**:** 89.0
MW: 318.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E-07	5.500E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.258E-07	4.000E-05	20	C053	0 0 0 0 0	
1.258E-07	4.000E-05	20	F071	1 1 2 1 1	
3.773E-07	1.200E-04	25	B083	2 2 1 2 2	particle size 5 µm
3.773E-07	1.200E-04	25	I308	0 0 0 0 0	
4.088E-09	1.300E-06	25	M134	1 2 1 1 1	
4.402E-08	1.400E-05	25	W025	1 0 1 1 1	
7.389E-07	2.350E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.415E-06	4.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
4.717E-09	1.500E-06	ns	M110	0 0 0 0 0	EFG
4.088E-09	1.300E-06	ns	M118	0 1 1 1 1	

3191. $C_{14}H_8O_2$

Anthraquinone
9,10-Anthraquinone
9,10-Dioxoanthracene
Corbit
Morkit
Hoelite
RN: 84-65-1 **MP** (°C)**:** 286
MW: 208.22 **BP** (°C)**:** 377

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-06	1.353E-03	25	E014	2 2 2 1 1	pH 7.3
3.000E-06	6.247E-04	ns	G077	0 0 0 0 1	

3192. $C_{14}H_8O_4$

Alizarin
Alizarine
C.I. Mordant red 11

RN: 72-48-0 **MP** (°C)**:** 290
MW: 240.22 **BP** (°C)**:** 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.123E-03	25	B333	0 0 0 0 0	*sic*
1.664E-03	3.998E-01	rt	D021	0 0 1 1 1	*sic*

3193. $C_{14}H_8O_4$

Quinizarin
1,4-Dihydroxyanthraquinone
C.I. Pigment violet 12

RN: 81-64-1 **MP** (°C)**:** 192
MW: 240.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-07	9.609E-05	25	B333	0 0 0 0 0	
6.000E-05	1.441E-02	98.59	M180	0 0 2 2 0	EFG
9.200E-05	2.210E-02	111.46	M180	0 0 2 2 0	EFG
1.100E-04	2.642E-02	117.47	M180	0 0 2 2 0	EFG
1.800E-04	4.324E-02	123.67	M180	0 0 2 2 0	EFG
2.000E-04	4.804E-02	126.84	M180	0 0 2 2 0	EFG
2.100E-04	5.045E-02	135.00	M180	0 0 2 2 0	EFG
4.900E-04	1.177E-01	141.78	M180	0 0 2 2 0	EFG
7.500E-04	1.802E-01	152.37	M180	0 0 2 2 0	EFG

3194. $C_{14}H_8O_5$

Purpurin
1,2,4-Trihydroxy-anthrachinon

RN: 81-54-9 **MP** (°C)**:**
MW: 256.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.405E-03	25	B333	0 0 0 0 0	

3195. $C_{14}H_8O_6$
Quinalizarin
1,2,5,8-Tetrahydroxyanthraquinone
9,10-Anthracenedione
Alizarine Bordeaux B
Mordant violet 26
RN: 81-61-8 **MP** (°C)**:**
MW: 272.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-06	2.586E-03	25	B333	0 0 0 0 0	

3196. $C_{14}H_8O_8S_2$
Anthraquinone-1,8-disulfonic acid
1,8-Disulfonic acid anthraquinone
Anthrachinon-disulfosaeure-(1,8)
1,8-Anthraquinone disulfonic acid
RN: 82-48-4 **MP** (°C)**:** 293
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3197. $C_{14}H_8O_8S_2$
1,6-Anthraquinone disulfonic acid
Anthraquinone-1,6-disulfonic acid
RN: 14486-58-9 **MP** (°C)**:** 216
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.357E+00	5.000E+02	18	F047	1 2 1 1 0	

3198. $C_{14}H_8O_8S_2$
1,5-Anthraquinone disulfonic acid
Anthraquinone-1,5-disulfonic acid
RN: 252967-17-2 **MP** (°C)**:** 310.0
MW: 368.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3199. $C_{14}H_9ClF_2N_2O_2$

Difluron
Diflubenzuron
TH 6040

RN: 35367-38-5 **MP** (°C)**:** 239
MW: 310.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.437E-07	2.000E-04	20	M161	1 0 0 0 0	
2.865E-07	8.900E-05	20	M402	0 0 0 0 0	
6.437E-07	2.000E-04	20	R303	1 0 0 0 0	
9.656E-07	3.000E-04	24	C105	2 1 2 2 2	
1.609E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
2.570E-07	7.986E-05	ns	R427	0 0 0 0 0	

3200. $C_{14}H_9ClF_3NO_2$

Efavirenz
8-Chloro-5-(2-cyclopropylethynyl)-5-(trifluoromethyl)-4-oxa-2-azabicyclo [4.4.0]deca-7,9,11-trien-3-one

RN: 154598-52-4 **MP** (°C)**:**
MW: 315.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	8.000E-03	ns	A426	0 0 0 0 0	intrinsic
3.168E-05	1.000E-02	ns	K444	0 0 0 0 0	

3201. $C_{14}H_9Cl_2NO_5$

Bifenox
5-(2,4-Dichlorphenoxy)-2-nitro-benzoic acid methyl ester
Modown 4 flowable
Modown

RN: 42576-02-3 **MP** (°C)**:** 85
MW: 342.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.461E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
1.023E-06	3.500E-04	ns	M161	0 0 0 0 1	
1.023E-06	3.501E-04	ns	R427	0 0 0 0 0	

3202. $C_{14}H_9Cl_5$

o,p′-DDT
1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2,2-trichloroethane
2,4′-DDT
2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1,1-trichloroethane
RN: 789-02-6 **MP** (°C)**:** 74.0
MW: 354.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.398E-07	8.500E-05	25	B083	2 2 1 2 1	particle size 5 µm
2.398E-07	8.500E-05	25	I308	0 0 0 0 0	
7.334E-08	2.600E-05	25	W025	1 0 2 2 1	
3.808E-07	1.350E-04	35	B083	2 2 1 2 2	particle size 5 µm
5.642E-07	2.000E-04	45	B083	2 2 1 2 2	particle size 5 µm

3203. $C_{14}H_9Cl_5$

p,p′-DDT
2,2-bis(*p*-Chlorophenyl)-1,1,1-trichloroethane
p,p′-TDEE
RN: 50-29-3 **MP** (°C)**:** 108.5
MW: 354.49 **BP** (°C)**:** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.385E-09	1.200E-06	0	G319	0 0 0 0 0	
1.664E-08	5.900E-06	2	B186	2 0 2 2 2	
4.796E-08	1.700E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.834E-07	6.500E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.800E-07	9.926E-05	18	G054	1 0 1 0 1	
1.410E-08	5.000E-06	20	C111	1 0 0 0 0	
1.410E-08	5.000E-06	20	C113	1 0 2 1 1	
1.128E-07	4.000E-05	20	E048	1 2 1 1 0	
2.172E-08	7.700E-06	20	F303	1 2 1 2 1	
2.172E-08	7.700E-06	20	W319	1 2 1 2 1	
1.552E-08	5.500E-06	24	C311	0 0 0 0 0	EFG
1.523E-08	5.400E-06	24	C313	0 0 0 0 0	
2.821E-09	1.000E-06	24	K069	2 0 0 1 1	
7.079E-08	2.510E-05	24.99	K436	0 0 0 0 0	
3.385E-09	1.200E-06	25	B036	1 1 0 1 1	
3.949E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 µm
7.052E-08	2.500E-05	25	B083	2 2 1 2 1	particle size 5 µm
4.796E-09	1.700E-06	25	B093	2 2 2 2 1	
1.055E-07	3.740E-05	25	B186	2 0 2 2 2	
9.168E-09	3.250E-06	25	F071	1 1 2 1 1	
3.385E-09	1.200E-06	25	M040	1 0 0 1 1	
3.385E-09	1.200E-06	25	M130	1 0 0 0 1	
2.821E-09	1.000E-06	25	P085	0 0 0 0 0	
1.552E-08	5.500E-06	25	W025	1 0 2 2 1	
3.385E-09	1.200E-06	26.70	L095	2 2 1 1 2	

(*continued*)

3203. $C_{14}H_9Cl_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-07	3.700E-05	35	B083	2 2 1 2 1	particle size 5 µm
7.334E-07	2.600E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.269E-07	4.500E-05	37.50	B186	2 0 2 2 2	
1.269E-07	4.500E-05	45	B083	2 2 1 2 1	particle size 5 µm
1.439E-06	5.100E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.552E-08	5.500E-06	ns	C318	0 0 0 0 0	
3.385E-09	1.200E-06	ns	I300	0 0 0 0 1	
4.796E-09	1.700E-06	ns	K138	0 0 0 0 2	
2.821E-09	1.000E-06	ns	M061	0 0 0 0 0	
3.103E-09	1.100E-06	ns	M110	0 0 0 0 0	EFG
5.642E-09	2.000E-06	ns	M138	0 0 0 0 0	
8.745E-09	3.100E-06	ns	M344	0 0 0 0 1	
2.821E-08	1.000E-05	ns	V414	0 0 0 0 0	
2.539E-07	9.000E-05	ns	V414	0 0 0 0 0	

3204. $C_{14}H_9Cl_5O$

Dicofol
4-Chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzenemethanol
4,4′-Dichloro-α-(trichloromethyl)benzhydrol
Acarin
Carbox
Cekudifol

RN: 115-32-2 **MP** (°C)**:** 79
MW: 370.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.563E-06	1.320E-03	25	W025	1 0 2 2 2	

3205. $C_{14}H_9F$

1-Fluoroanthracene

RN: 7651-80-1 **MP** (°C)**:**
MW: 196.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-06	2.600E-04	ns	M344	0 0 0 0 2	

3206. $C_{14}H_9NO_2$
2-Aminoanthraquinone
2-Amino-9,10-anthracenedione
2-Amino-9,10-anthraquinone
Aminoanthraquinone
AAQ
RN: 117-79-3 **MP** (°C)**:** 310
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-07	1.630E-04	25	B333	0 0 0 0 0	

3207. $C_{14}H_9NO_2$
1-Aminoanthraquinone
1-Amino-9,10-anthracenedione
1-Amino-9,10-anthraquinone
RN: 82-45-1 **MP** (°C)**:** 254
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.125E-04	25	B333	0 0 0 0 0	

3208. $C_{14}H_9NO_2$
2-Phenyl-3,1-benzoxazin-4-one
Bentranil
Linarotox
Linurotox
RN: 1022-46-4 **MP** (°C)**:** 123.5
MW: 223.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.464E-05	5.500E-03	20	M161	1 0 0 0 0	

3209. $C_{14}H_9NO_2S$
4-Benzoyl phenylisothiocyanate
4-Isothiocyanatobenzophenone
RN: 26328-59-6 **MP** (°C)**:**
MW: 255.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	3.574E-03	25	K032	2 2 0 1 1	

3210. $C_{14}H_9NO_3$

1-Amino-4-hydroxyanthraquinone
C.I. Disperse red 15
Disperse red 15
Celliton fast pink B

RN: 116-85-8 **MP** (°C)**:** 208
MW: 239.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.871E-04	25	B333	0 0 0 0 0	
1.129E-05	2.700E-03	60	P313	0 0 0 0 0	average of 2
1.797E-05	4.300E-03	70	P313	0 0 0 0 0	average of 2
2.320E-05	5.550E-03	80	P313	0 0 0 0 0	average of 2
4.828E-05	1.155E-02	90	P313	0 0 0 0 0	average of 2
1.500E-04	3.588E-02	98.59	M180	0 0 2 2 0	EFG
2.500E-04	5.981E-02	111.46	M180	0 0 2 2 0	EFG
3.000E-04	7.177E-02	114.44	M180	0 0 2 2 0	EFG
4.500E-04	1.077E-01	122.10	M180	0 0 2 2 0	EFG
6.000E-04	1.435E-01	126.84	M180	0 0 2 2 0	EFG
6.500E-04	1.555E-01	130.07	M180	0 0 2 2 0	EFG
1.500E-03	3.588E-01	152.37	M180	0 0 2 2 0	EFG

3211. $C_{14}H_{10}$

Phenanthrene
Phenanthracene

RN: 85-01-8 **MP** (°C)**:** 100
MW: 178.24 **BP** (°C)**:** 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.462E-06	2.607E-04	-.7	N053	1 0 0 1 0	EFG
1.970E-06	3.511E-04	4.00	M082	1 1 1 2 2	
1.970E-06	3.511E-04	4.00	M151	2 1 2 2 2	
2.027E-06	3.613E-04	4.04	M183	1 2 1 1 2	
2.265E-06	4.037E-04	4.62	N053	1 0 0 1 0	EFG
2.373E-06	4.230E-04	8.50	M063	2 1 2 2 2	
2.370E-06	4.224E-04	8.50	M082	1 1 1 2 2	
2.370E-06	4.224E-04	8.50	M151	2 1 2 2 2	
2.375E-06	4.233E-04	8.54	M183	1 2 1 1 2	
2.626E-06	4.680E-04	10.00	M063	2 1 2 2 2	
2.630E-06	4.688E-04	10.00	M082	1 1 1 2 2	
2.630E-06	4.688E-04	10.00	M151	2 1 2 2 2	
2.628E-06	4.684E-04	10.04	M183	1 2 1 1 2	
3.055E-06	5.446E-04	10.13	N053	1 0 0 1 0	EFG
2.873E-06	5.120E-04	12.50	M063	2 1 2 2 2	
2.870E-06	5.115E-04	12.50	M082	1 1 1 2 2	
2.870E-06	5.115E-04	12.50	M151	2 1 2 2 2	
2.875E-06	5.124E-04	12.54	M183	1 2 1 1 2	
3.759E-06	6.700E-04	14.20	N053	1 0 0 1 0	EFG
3.372E-06	6.010E-04	15.00	M063	2 1 2 2 2	

(*continued*)

3211. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.370E-06	6.007E-04	15.00	M082	1 1 1 2 2	
3.370E-06	6.007E-04	15.00	M151	2 1 2 2 2	
3.375E-06	6.015E-04	15.04	M183	1 2 1 1 2	
1.500E-05	2.674E-03	20	E025	1 0 2 2 2	
6.200E-06	1.105E-03	20	H306	1 0 1 2 1	
5.061E-06	9.020E-04	20	V416	0 0 0 0 0	
4.420E-06	7.878E-04	20.00	M082	1 1 1 2 2	
4.420E-06	7.878E-04	20.00	M151	2 1 2 2 2	
4.419E-06	7.877E-04	20.04	M183	1 2 1 1 2	
4.578E-06	8.160E-04	21.00	M063	2 1 2 2 2	
4.580E-06	8.163E-04	21.00	M082	1 1 1 2 2	
4.580E-06	8.163E-04	21.00	M151	2 1 2 2 2	
4.582E-06	8.167E-04	21.04	M183	1 2 1 1 2	
7.200E-06	1.283E-03	22	A413	2 0 2 2 1	
5.582E-06	9.950E-04	24.30	M063	2 1 2 2 2	
5.360E-06	9.553E-04	24.30	M082	1 1 1 2 2	
5.360E-06	9.553E-04	24.30	M151	2 1 2 2 2	
5.363E-06	9.558E-04	24.34	M183	1 2 1 1 2	
6.284E-06	1.120E-03	24.60	W003	2 2 2 2 2	average of 2
5.577E-06	9.940E-04	25	A001	1 2 2 2 2	
6.059E-06	1.080E-03	25	B319	2 0 1 2 1	
4.617E-06	8.230E-04	25	D406	1 2 2 2 2	
6.003E-06	1.070E-03	25	E004	2 1 2 2 2	
9.000E-06	1.604E-03	25	K001	2 2 2 2 0	
5.611E-06	1.000E-03	25	L332	1 1 1 1 1	
7.238E-06	1.290E-03	25	M064	1 1 2 2 2	
6.620E-06	1.180E-03	25	M342	1 0 1 1 2	
3.815E-06	6.800E-04	25	P340	0 0 0 0 0	
7.278E-06	1.297E-03	25	T066	1 0 0 0 2	
5.610E-06	9.999E-04	25	W300	2 2 2 2 2	
5.622E-06	1.002E-03	25.00	M151	2 1 1 2 2	
6.800E-06	1.212E-03	25.04	V013	2 2 2 2 2	
5.690E-06	1.014E-03	25.35	N053	1 0 0 1 0	EFG
8.977E-06	1.600E-03	27	D003	1 0 0 1 1	
9.257E-06	1.650E-03	27	D043	2 0 0 0 2	average of 2
7.854E-06	1.400E-03	28.95	N053	1 0 0 1 0	EFG
6.845E-06	1.220E-03	29	M071	2 2 2 2 2	
6.845E-06	1.220E-03	29.00	M151	2 1 1 2 2	
7.165E-06	1.277E-03	29.90	M063	2 1 2 2 2	
7.160E-06	1.276E-03	29.90	M082	1 1 1 2 2	
7.160E-06	1.276E-03	29.90	M151	2 1 2 2 2	
8.360E-06	1.490E-03	29.90	W003	2 2 2 2 2	
6.867E-06	1.224E-03	29.94	M183	1 2 1 1 2	
8.304E-06	1.480E-03	30.30	W003	2 2 2 2 2	average of 2
1.035E-05	1.845E-03	34.53	N053	1 0 0 1 0	EFG
1.375E-05	2.450E-03	38.40	W003	2 2 2 2 2	average of 2
1.440E-05	2.566E-03	40	V416	0 0 0 0 0	
1.274E-05	2.270E-03	40.10	W003	2 2 2 2 2	average of 3
2.171E-05	3.870E-03	47.50	W003	2 2 2 2 2	average of 3

(*continued*)

3211. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.429E-05	4.330E-03	50.10	W003	2 2 2 2 2	average of 3
2.289E-05	4.080E-03	50.20	W003	2 2 2 2 2	average of 3
3.164E-05	5.640E-03	54.70	W003	2 2 2 2 2	average of 3
4.034E-05	7.190E-03	59.20	W003	2 2 2 2 2	average of 3
3.559E-05	6.344E-03	60	V416	0 0 0 0 0	
4.096E-05	7.300E-03	60.50	W003	2 2 2 2 1	average of 3
5.498E-05	9.800E-03	65.10	W003	2 2 2 2 1	average of 3
7.013E-05	1.250E-02	70.70	W003	2 2 2 2 2	average of 3
7.238E-05	1.290E-02	71.90	W003	2 2 2 2 2	
8.528E-05	1.520E-02	73.40	W003	2 2 2 2 2	
7.238E-06	1.290E-03	ns	H123	0 0 0 0 0	
7.238E-06	1.290E-03	ns	K304	0 0 0 0 2	
7.238E-06	1.290E-03	ns	M344	0 0 0 0 2	
1.500E-05	2.674E-03	ns	W005	0 0 1 2 1	

3212. $C_{14}H_{10}$

Anthracene
Paranaphthalene
Anthracin
Green oil
Anthraxcene

RN: 120-12-7 **MP** (°C)**:** 218
MW: 178.24 **BP** (°C)**:** 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.125E-08	1.270E-05	5.20	M063	2 1 2 2 2	
7.100E-08	1.265E-05	5.20	M082	1 1 1 2 1	
7.100E-08	1.265E-05	5.20	M151	2 1 2 2 1	
7.133E-08	1.271E-05	5.24	M183	1 2 1 1 2	
9.818E-08	1.750E-05	10.00	M063	2 1 2 2 2	
9.800E-08	1.747E-05	10.00	M082	1 1 1 2 1	
9.800E-08	1.747E-05	10.00	M151	2 1 2 2 1	
9.828E-08	1.752E-05	10.04	M183	1 2 1 1 2	
9.094E-08	1.621E-05	9.74	M183	1 2 1 1 2	
1.246E-07	2.220E-05	14.10	M063	2 1 2 2 2	
1.250E-07	2.228E-05	14.10	M082	1 1 1 2 2	
1.250E-07	2.228E-05	14.10	M151	2 1 2 2 2	
1.247E-07	2.223E-05	14.14	M183	1 2 1 1 2	
1.212E-07	2.160E-05	15	B385	0 0 0 0 0	
1.409E-07	2.512E-05	16.64	M183	1 2 1 1 2	
1.633E-07	2.910E-05	18.30	M063	2 1 2 2 2	
1.630E-07	2.905E-05	18.30	M082	1 1 1 2 2	
1.630E-07	2.905E-05	18.30	M151	2 1 2 2 2	
1.634E-07	2.912E-05	18.34	M183	1 2 1 1 2	
2.400E-07	4.278E-05	20	E009	1 0 0 0 1	
2.240E-07	3.992E-05	20	E025	1 0 2 2 2	
1.851E-07	3.300E-05	20	H300	1 1 2 2 1	

(*continued*)

3212. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.087E-07	3.720E-05	22.40	M063	2 1 2 2 2	
2.090E-07	3.725E-05	22.40	M082	1 1 1 2 2	
2.090E-07	3.725E-05	22.40	M151	2 1 2 2 2	
2.089E-07	3.723E-05	22.44	M183	1 2 1 1 2	
2.974E-07	5.300E-05	22.5	G301	0 0 0 0 0	
3.927E-07	7.000E-05	23	P332	0 0 0 0 0	
3.927E-07	7.000E-05	23	P339	0 0 0 0 0	
2.123E-07	3.784E-05	23.24	M183	1 2 1 1 2	
2.435E-07	4.340E-05	24.60	M063	2 1 2 2 2	
2.440E-07	4.349E-05	24.60	M082	1 1 1 2 2	
2.440E-07	4.349E-05	24.60	M151	2 1 2 2 2	
2.437E-07	4.344E-05	24.64	M183	1 2 1 1 2	
2.500E-07	4.456E-05	25	A325	2 1 2 2 1	
2.188E-07	3.900E-05	25	B319	2 0 1 2 1	average of 2
2.174E-07	3.875E-05	25	B385	0 0 0 0 0	
5.218E-07	9.300E-05	25	D406	1 2 2 2 2	
4.470E-07	7.967E-05	25	K001	2 2 2 2 2	
3.800E-07	6.773E-05	25	K123	1 0 2 2 1	
4.152E-07	7.400E-05	25	L301	1 1 2 2 2	
3.927E-07	7.000E-05	25	L332	1 1 1 1 2	
4.096E-07	7.300E-05	25	M064	1 1 2 2 1	
4.100E-06	7.308E-04	25	M342	1 0 1 1 2	
1.683E-07	3.000E-05	25	S227	1 2 1 1 1	
4.211E-07	7.506E-05	25	T066	1 0 0 0 2	
2.500E-07	4.456E-05	25	W300	2 2 2 2 2	
2.502E-07	4.460E-05	25.00	M151	2 1 1 2 2	
4.208E-07	7.500E-05	27	D003	1 0 0 1 1	
3.125E-07	5.570E-05	28.70	M063	2 1 2 2 2	
3.130E-07	5.579E-05	28.70	M082	1 1 1 2 2	
3.130E-07	5.579E-05	28.70	M151	2 1 2 2 2	
3.128E-07	5.575E-05	28.74	M183	1 2 1 1 2	
3.198E-07	5.700E-05	29	M071	2 2 2 2 2	
3.198E-07	5.700E-05	29.00	M151	2 1 1 2 2	
3.212E-07	5.724E-05	29.34	M183	1 2 1 1 2	
3.512E-07	6.260E-05	35	B385	0 0 0 0 0	
6.845E-07	1.220E-04	35.40	W003	2 2 2 2 2	average of 3
8.416E-07	1.500E-04	39.30	W003	2 2 2 2 2	average of 3
1.167E-06	2.080E-04	44.70	W003	2 2 2 2 2	average of 3
1.565E-06	2.790E-04	47.50	W003	2 2 2 2 2	
1.683E-06	3.000E-04	50.10	W003	2 2 2 2 2	average of 3
2.211E-06	3.940E-04	54.70	W003	2 2 2 2 2	average of 3
2.794E-06	4.980E-04	59.20	W003	2 2 2 2 2	average of 3
3.703E-06	6.600E-04	64.50	W003	2 2 2 2 1	average of 3
3.703E-06	6.600E-04	65.10	W003	2 2 2 2 1	average of 3
5.162E-06	9.200E-04	69.80	W003	2 2 2 2 1	
5.274E-06	9.400E-04	70.70	W003	2 2 2 2 1	average of 3
5.106E-06	9.100E-04	71.90	W003	2 2 2 2 2	
6.677E-06	1.190E-03	74.70	W003	2 2 2 2 2	average of 3
2.356E-07	4.200E-05	ns	H123	0 0 0 0 0	

(*continued*)

3212. $C_{14}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	3.208E-05	ns	H306	1 0 1 2 1	
4.096E-07	7.300E-05	ns	K304	0 0 0 0 1	
4.096E-07	7.300E-05	ns	M344	0 0 0 0 2	
5.000E-07	8.912E-05	ns	W005	0 0 1 2 0	

3213. $C_{14}H_{10}Cl_2O_3$

Fenclofenac
Benzeneacetic acid, 2-(2,4-dichlorophenoxy)-
RX 67408

RN: 34645-84-6 **MP** (°C)**:** 136
MW: 297.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.840E-05	8.439E-03	25	C314	0 0 0 0 0	
2.827E-05	8.400E-03	25	C314	0 0 0 0 0	

3214. $C_{14}H_{10}Cl_4$

DDD
1,1-Dichloro-2,2-bis(*p*-chlorophenyl)ethane
p,p′-TDE
Dichlorodiphenyldichloroethane

RN: 72-54-8 **MP** (°C)**:** 109.5
MW: 320.05 **BP** (°C)**:** 193

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.812E-07	9.000E-05	25	B083	2 2 1 2 1	particle size 5 µm
6.249E-08	2.000E-05	25	W025	1 0 2 2 1	
4.687E-07	1.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
7.499E-07	2.400E-04	45	B083	2 2 1 2 2	particle size 5 µm
9.374E-09	3.000E-06	ns	M110	0 0 0 0 0	EFG

3215. $C_{14}H_{10}Cl_4$

1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane
o,p′-DDD

RN: 53-19-0 **MP** (°C)**:** 76
MW: 320.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.875E-07	6.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
3.125E-07	1.000E-04	25	B083	2 2 1 2 2	particle size 5 µm
8.749E-07	2.800E-04	35	B083	2 2 1 2 2	particle size 5 µm
9.842E-07	3.150E-04	45	B083	2 2 1 2 2	particle size 5 µm

3216. $C_{14}H_{10}F_3NO_2$

Flufenamic acid
N-(α,α,α-Trifluoro-*m*-tolyl)anthranilic acid
N-(3-Trifluoromethylphenyl)anthranilic acid
RN: 530-78-9 **MP** (°C)**:** 132–135
MW: 281.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-06	1.094E-03	25	G085	2 0 0 0 0	EFG
4.000E-05	1.125E-02	25	I007	1 2 2 2 0	EFG
1.031E-04	2.900E-02	30	D015	2 0 1 1 0	EFG
6.670E-06	1.876E-03	35	G085	2 0 0 0 0	EFG
6.200E-04	1.744E-01	35	H091	1 2 2 2 1	*sic*
2.133E-04	6.000E-02	37	D015	2 0 1 1 0	EFG
3.556E-05	1.000E-02	rt	H302	0 0 2 1 2	intrinsic

3217. $C_{14}H_{10}N_2O_2$

C.I. Disperse violet 1
1,4-Diamino-9,10-anthraquinone
Acetate red violet R
Acetoquinone light heliotrope NL
Supracet brilliant violet 3R
Violet 14447
RN: 128-95-0 **MP** (°C)**:** 275
MW: 238.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-07	2.287E-04	25	B333	0 0 0 0 0	

3218. $C_{14}H_{10}N_2O_6$

Dipentum
Olsalazine
RN: 15722-48-2 **MP** (°C)**:**
MW: 302.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.149E-05	25	D311	0 0 0 0 0	0.1M NaCl

3219. $C_{14}H_{10}O$

2-Anthranol
2-Anthrol
RN: 613-14-9 **MP** (°C)**:**
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-04	9.167E-02	25	L085	1 2 0 1 2	

3220. $C_{14}H_{10}O$

1-Anthranol
1-Anthrol
Anthranol

RN: 529-86-2 **MP** (°C)**:** 152
MW: 194.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.593E-02	25	L085	1 2 0 1 2	

3221. $C_{14}H_{10}O_3$

Diphenyleneglycollic acid

RN: **MP** (°C)**:**
MW: 226.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.082E-02	2.448E+00	25	K040	1 0 2 1 2	

3222. $C_{14}H_{10}O_4$

Diphenic acid
1,1′-Biphenyl-2,2′-dicarboxylic acid
2,2′-Biphenyldicarboxylic acid

RN: 482-05-3 **MP** (°C)**:** 228
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	1.260E+00	25	K040	1 0 2 1 2	

3223. $C_{14}H_{10}O_4$

Benzoyl peroxide
Benzoyl-peroxid

RN: 94-36-0 **MP** (°C)**:** 105
MW: 242.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-07	1.550E-04	rt	C342	0 0 0 0 0	

3224. $C_{14}H_{10}O_5$

Gentisin
9H-Xanthen-9-one, 1,7-dihydroxy-3-methoxy-
Gentianic acid
Gentianin

RN: 437-50-3 **MP** (°C)**:** 266.5
MW: 258.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-03	3.000E-01	16	F300	1 0 0 0 2	

3225. $C_{14}H_{10}O_9$

Digallic acid
m-Digallic acid
m-Digallussaeure

RN: 536-08-3 **MP** (°C)**:**
MW: 322.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.552E-03	5.000E-01	25	F300	1 0 0 0 0	
5.896E-02	1.900E+01	100	F300	1 0 0 0 1	

3226. $C_{14}H_{11}ClNO_2$

7-Chloro-5,11-dihydrodibenz[b,e][1,4]oxazepine-5-carboxamide

RN: **MP** (°C)**:**
MW: 260.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.534E-04	4.000E-02	37	G020	1 0 0 0 1	

3227. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′chloro-2-hydroxy-5-nitrobenzanilide
Benzamide, *N*-(3-chloro-2-methyphenyl)-2-hydroxy-5-nitro-

RN: 213460-66-3 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-05	3.379E-03	25	D400	2 0 0 1 2	

3228. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-5′-chloro-2-hydroxy-5-nitrobenzanilide
Benzamide, *N*-(5-chloro-2-methylphenyl)-2-hydroxy-5-nitro-
RN: 213460-65-2 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.534E-06	2.311E-03	25	D400	2 0 0 1 2	

3229. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′-chloro-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(3-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 73544-88-4 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:** 324.7–408.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3230. $C_{14}H_{11}ClN_2O_4$

2′-Methyl-3′-chloro-2-hydroxy-3nitrobenzanilide
Benzamide, *N*-(5-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 213460-62-9 **MP** (°C)**:**
MW: 306.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3231. $C_{14}H_{11}ClN_2O_4S$

Chlorthalidone
2-Chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isoindol-1-yl)benzenesulfonamide
Hygroton
Thalitone
Chlortalidone
RN: 77-36-1 **MP** (°C)**:**
MW: 338.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.542E-04	1.200E-01	25	P312	0 0 0 0 0	
4.510E-04	1.528E-01	ns	I304	0 0 0 0 0	

3232. $C_{14}H_{11}Cl_2NO_2$

Diclofenac
2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid
RN: 15307-86-5 **MP** (°C)**:** 157
MW: 296.16 **BP** (°C)**:** 412

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.317E-06	1.278E-03	30	P438	0 0 0 0 0	pH 2.0
1.182E-05	3.500E-03	32	C411	2 1 1 2 1	
4.478E-06	1.326E-03	33	P438	0 0 0 0 0	pH 2.0
5.117E-06	1.515E-03	37	P438	0 0 0 0 0	pH 2.0
5.389E-06	1.596E-03	39.5	P438	0 0 0 0 0	pH 2.0
5.822E-06	1.724E-03	42	P438	0 0 0 0 0	pH 2.0

3233. $C_{14}H_{11}Cl_3O_2$

2,2-bis(-*p*-Hydroxyphenyl)-1,1,1-trichloroethylene
Hydroxychlor
p,p′-Hydroxy-DDT
RN: 2971-36-0 **MP** (°C)**:** 194
MW: 317.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-04	7.600E-02	ns	K117	0 1 2 1 1	

3234. $C_{14}H_{11}FN_2O_5$

1-Acetoxymethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Acetoxymethyl-3-benzoyl-5-fluorouracil
RN: 97096-67-8 **MP** (°C)**:** 127–128
MW: 306.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.400E-01	22	B321	0 0 0 0 0	pH 4.0

3235. $C_{14}H_{11}N$

2-Aminoanthracene
2-Anthrylamine
β-Aminoanthracene
2-Anthracenamine
2-Anthramine
Anthracene amine
RN: 613-13-8 **MP** (°C)**:** 238
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-06	1.300E-03	24	H106	1 0 2 2 2	
6.727E-09	1.300E-06	ns	M349	0 2 1 1 2	

3236. $C_{14}H_{11}N$
Acetonitrile, diphenyl-
Diphenatrile
RN: 86-29-3 **MP** (°C)**:** 74
MW: 193.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-03	2.200E-01	ns	B185	0 0 0 0 0	

3237. $C_{14}H_{11}NO_2$
N-Benzoylbenzamide
Dibenzamid
RN: 614-28-8 **MP** (°C)**:** 152
MW: 225.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.327E-03	1.200E+00	15	F300	1 0 0 0 1	

3238. $C_{14}H_{11}N_3O_2$
Salicylolhydrazone of picolinealdehyde
RN: **MP** (°C)**:**
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.897E-04	2.000E-01	ns	G089	0 1 2 0 1	

3239. $C_{14}H_{12}$
1-Methylfluorene
1-Methyl-9H-fluorene
RN: 1730-37-6 **MP** (°C)**:** 87
MW: 180.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-06	1.090E-03	25	B319	2 0 1 2 2	
6.060E-06	1.092E-03	25	M342	1 0 1 1 2	

3240. $C_{14}H_{12}$
1,1-Diphenylethene
1,1-Diphenylethylene
RN: 530-48-3 **MP** (°C)**:** 8.2
MW: 180.25 **BP** (°C)**:** 277

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.662E-05	6.600E-03	25	A002	1 0 1 1 1	

3241. $C_{14}H_{12}$

9,10-Dihydroanthracene

RN: 613-31-0 **MP** (°C)**:** 104–107
MW: 180.25 **BP** (°C)**:** 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.578E-06	4.646E-04	4.96	R423	0 0 0 0 0	
2.622E-06	4.727E-04	5.85	R423	0 0 0 0 0	
2.917E-06	5.257E-04	7.95	R423	0 0 0 0 0	
3.317E-06	5.978E-04	10.95	R423	0 0 0 0 0	
3.556E-06	6.409E-04	12.05	R423	0 0 0 0 0	
4.261E-06	7.681E-04	14.95	R423	0 0 0 0 0	
4.961E-06	8.942E-04	18.00	R423	0 0 0 0 0	
5.811E-06	1.047E-03	20.96	R423	0 0 0 0 0	
7.389E-06	1.332E-03	24.59	R423	0 0 0 0 0	
8.011E-06	1.444E-03	26.59	R423	0 0 0 0 0	
9.400E-06	1.694E-03	29.05	R423	0 0 0 0 0	
1.114E-05	2.009E-03	32.66	R423	0 0 0 0 0	
1.288E-05	2.321E-03	36.28	R423	0 0 0 0 0	
1.498E-05	2.701E-03	40.01	R423	0 0 0 0 0	

3242. $C_{14}H_{12}$

trans-Stilbene
trans-Diphenylethylene
1,2-Diphenylethene
trans-1,2-Diphenylethylene
trans-α, β-Diphenylethylene
Toluylene

RN: 103-30-0 **MP** (°C)**:** 124
MW: 180.25 **BP** (°C)**:** 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.609E-06	2.900E-04	25	A002	1 0 1 1 1	

3243. $C_{14}H_{12}F_3NO_4S_2$

Perfluidone
Methyl-4-(phenylsulfonyl)trifluoromethanesulfonanilide
1,1,1-Trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide
Destun
MBR 8251
Trifluoro-*N*-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide

RN: 37924-13-3 **MP** (°C)**:** 143
MW: 379.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.582E-04	6.000E-02	22	G306	1 0 0 0 1	
1.582E-04	6.000E-02	22	M161	1 0 0 0 1	

3244. $C_{14}H_{12}N_2O_4$
4′-Methyl-2-hydroxy-5-nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(4-methylphenyl)--nitro-
RN: 68507-96-0 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-05	3.846E-03	25	D400	2 0 0 1 2	

3245. $C_{14}H_{12}N_2O_4$
4′-Methyl-2-hydroxy-3-nitrobenzanilide
Benzamide,2-hydroxy-*N*-(4-methylpheyl)-3-nitro-
RN: 68507-90-4 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:** 305.7–389.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E-05	8.356E-03	25	D400	2 0 0 1 2	

3246. $C_{14}H_{12}N_2O_4$
2′-Methyl-2-hydroxy-3-nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(2-methylphenyl)-3-nitro-
RN: 68507-89-1 **MP** (°C)**:**
MW: 272.26 **BP** (°C)**:** 302–384.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.818E-05	7.673E-03	25	D400	2 0 0 1 2	

3247. $C_{14}H_{12}N_2O_5$
4′-Methoxy-2-hydroxy-5nitrobenzanilide
p-Salicylanisidide, 5-nitro-
Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-5-nitro-
RN: 68507-94-8 **MP** (°C)**:**
MW: 288.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-05	5.556E-03	25	D400	2 0 0 1 2	

3248. $C_{14}H_{12}N_2O_5$
4′-Methoxy-2-hydroxy-3nitrobenzanilide
Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-3-nitro-
RN: 68507-88-0 **MP** (°C)**:**
MW: 288.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.532E-05	1.018E-02	25	D400	2 0 0 1 2	

3249. $C_{14}H_{12}N_2S$

2-(4-Aminophenyl)-6-methyl-benzothiazole
Dehydrothio-*N*-toluidin
Dehydrothio-*N*-toluidine

RN: 92-36-4 **MP** (°C)**:** 194.8
MW: 240.33 **BP** (°C)**:** 434

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.080E-04	5.000E-02	100	F300	1 0 0 0 0	

3250. $C_{14}H_{12}N_4O_2$

C.I. Disperse blue 1
9,10-Anthracenedione, 1,4,5,8-tetraamino-

RN: 2475-45-8 **MP** (°C)**:** 332
MW: 268.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.683E-05	25	B333	0 0 0 0 0	

3251. $C_{14}H_{12}O_2$

4-Biphenylacetic acid
Felbinac

RN: 5728-52-9 **MP** (°C)**:**
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.927E-02	25	P344	0 0 0 0 0	EFG

3252. $C_{14}H_{12}O_2$

Benzoin
2-Hydroxy-1,2-diphenylethanone
Benzoylphenylcarbinol
2-Hydroxy-2-phenylacetophenone
Hydroxy-2-phenyl acetophenone

RN: 579-44-2 **MP** (°C)**:** 137
MW: 212.25 **BP** (°C)**:** 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	3.000E-01	25	F300	1 0 0 0 0	
1.413E-03	2.999E-01	rt	D021	0 0 1 1 0	

3253. $C_{14}H_{12}O_2$

Benzyl benzoate
Ascabin
Scabagen
Benzoic acid phenylmethyl ester
Benylate
Phenylmethyl benzoate

RN: 120-51-4 **MP** (°C)**:** 19
MW: 212.25 **BP** (°C)**:** 323

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.225E-04	2.600E-02	15	H069	1 0 1 1 1	
6.960E-03	1.477E+00	30	M444	0 0 0 0 0	
7.020E-03	1.490E+00	40	M444	0 0 0 0 0	
7.150E-03	1.518E+00	50	M444	0 0 0 0 0	
7.230E-03	1.535E+00	60	M444	0 0 0 0 0	

3254. $C_{14}H_{12}O_2$

Diphenylacetic acid
Diphenyl-essigsaeure

RN: 117-34-0 **MP** (°C)**:** 148
MW: 212.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.274E-01	25	K040	1 0 2 1 2	

3255. $C_{14}H_{12}O_3$

Benzilic acid
2,2-Diphenyl-2-hydroxyacetic acid
Diphenylglycolic acid
Benzeneacetic acid, α-hydroxy-α-phenyl-
2-Hydroxy-2,2-diphenylethanoic acid

RN: 76-93-7 **MP** (°C)**:** 150
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-03	1.755E+00	25	K040	1 0 2 1 2	
6.190E-03	1.413E+00	25	L050	2 0 1 2 2	

3256. $C_{14}H_{12}O_3$

Benzylparaben
Benzyl 4-hydroxybenzoate
Phenylmethyl ester

RN: 94-18-8 **MP** (°C)**:**
MW: 228.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.200E-02	25	P013	0 0 0 0 0	

3257. $C_{14}H_{12}O_5$

Khellin
Amicardine

RN: 82-02-0 **MP** (°C)**:** 154.5
MW: 260.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-01	2.472E+02	25	E312	0 0 0 0 0	EFG, *sic*
1.153E-04	3.000E-02	25	J028	1 2 0 2 0	
7.000E-04	1.822E-01	30	E012	1 2 1 1 0	
1.300E-03	3.383E-01	42	E012	1 2 1 1 0	

3258. $C_{14}H_{13}ClN_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-

RN: 133627-12-0 **MP** (°C)**:**
MW: 288.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.691E-05	2.221E-02	ns	M381	0 1 1 1 2	pH 7.0

3259. $C_{14}H_{13}NO_6$

Benzoic acid, 2-(acetyloxy)-, (2,5-dioxo-1-pyrrolidinyl)methyl ester
Salicylic acid acetate, ester with *N*-(hydroxymethyl)succinimide

RN: 32620-72-7 **MP** (°C)**:** 117.5
MW: 291.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.717E-03	5.000E-01	21	N335	0 0 0 0 0	

3260. $C_{14}H_{13}N_2$
4,7-Dimethyl-1,10-phenanthroline
4,7-Dimethyl-*o*-phenanthroline
RN: 3248-05-3 **MP** (°C)**:** 193
MW: 209.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.239E-02	25.04	B094	1 2 1 2 2	

3261. $C_{14}H_{13}N_3O_2$
Pyrido[2,3-b][1,5]benzoxazepin-5(6H)-one, 3-amino-6,9-dimethyl-
RN: 134894-45-4 **MP** (°C)**:**
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.057E-04	2.312E-01	ns	M381	0 1 1 1 2	pH 7.0

3262. $C_{14}H_{13}N_3O_4S_2$
Meloxicam
RN: 71125-38-7 **MP** (°C)**:**
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	2.284E-02	25	C434	0 0 0 0 0	pH 6.0
3.415E-05	1.200E-02	25	S415	0 0 0 0 0	
9.500E-05	3.338E-02	30	C434	0 0 0 0 0	pH 6.0
1.550E-05	5.447E-03	37	C434	0 0 0 0 0	pH 6.0
3.699E-06	1.300E-03	37	Y421	0 0 0 0 0	
2.800E-05	9.839E-03	45	C434	0 0 0 0 0	pH 6.0

3263. $C_{14}H_{14}$
4,4′-Dimethylbiphenyl
4,4′-Dimethyl-1,1′-biphenyl
p,p′-Bitoluene
RN: 613-33-2 **MP** (°C)**:** 125.0
MW: 182.27 **BP** (°C)**:** 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.770E-07	6.871E-05	4.0	D330	2 2 1 2 2	
9.590E-07	1.748E-04	25.0	D330	2 2 1 2 2	
2.420E-06	4.411E-04	40.0	D330	2 2 1 2 2	

3264. $C_{14}H_{14}$

Bibenzyl
1,2-Diphenylethane
Benzene, 1,1′-(1,2-ethanediyl)*bis*-
RN: 103-29-7 **MP** (°C)**:** 52.0
MW: 182.27 **BP** (°C)**:** 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.359E-05	4.300E-03	25	A002	1 0 1 1 1	

3265. $C_{14}H_{14}NO_4PS$

EPN
Ethyl *O*-(*p*-nitrophenyl) phenylphosphonothionate
O-Ethyl *O*-*p*-nitrophenyl benzenephosphonothioate
Ethyl *O*-(*p*-nitrophenyl) benzenethiophosphonate
RN: 2104-64-5 **MP** (°C)**:** 36
MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-06	3.113E-03	22	K137	1 1 2 1 0	

3266. $C_{14}H_{14}N_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl
RN: 132312-85-7 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-03	6.100E-01	ns	M381	0 1 1 1 2	pH 7.0

3267. $C_{14}H_{14}N_4O_2$

Dis. A. 7
RN: 2491-74-9 **MP** (°C)**:** 236
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-09	5.406E-07	25	B333	0 0 0 0 0	

3268. $C_{14}H_{14}N_4O_2$

Dye II
4-[[(4-Dimethylamino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-07	2.108E-04	84.10	B198	1 2 1 1 1	
2.040E-06	5.514E-04	97.40	B198	1 2 1 1 2	

3269. $C_{14}H_{14}N_4O_4$

β,γ-Dihydroxypropyltheophylline

RN: 180262-60-6 **MP** (°C)**:**

MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.007E-01	9.091E+01	ns	J025	0 0 0 0 1	

3270. $C_{14}H_{14}N_4S$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepine-6-thione, 11-ethyl-5,11-dihydro-5-methyl

RN: 134698-27-4 **MP** (°C)**:**

MW: 270.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-05	6.280E-03	ns	M381	0 1 1 1 2	pH 7.0

3271. $C_{14}H_{14}O$

6-Benzyl-*m*-cresol

Phenol, 5-methyl-2-(phenylmethyl)-

RN: 30091-04-4 **MP** (°C)**:**

MW: 198.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-04	2.857E-02	25	L021	1 0 0 0 0	

3272. $C_{14}H_{14}O$

DL-1,2-Diphenylethanol

DL-1,2-Diphenyl-aethanol

RN: 614-29-9 **MP** (°C)**:** 67

MW: 198.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-03	6.000E-01	100	F300	1 0 0 0 0	

3273. $C_{14}H_{14}O_2$

DL-Hydrobenzoin

Hydrobenzoin

RN: 27134-24-3 **MP** (°C)**:** 139

MW: 214.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E-02	2.500E+00	15	F300	1 0 0 0 1	
8.867E-03	1.900E+00	15	F300	1 0 0 0 1	
6.021E-02	1.290E+01	100	F300	1 0 0 0 2	

3274. $C_{14}H_{14}O_3$

Pindone
2-Pivaloylindandione-1,3
RN: 83-26-1 **MP** (°C)**:** 109
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-05	1.800E-02	25	M061	1 0 0 0 1	
7.817E-05	1.800E-02	25	M161	1 0 0 0 1	

3275. $C_{14}H_{14}O_3$

Naproxen
6-Methoxy-α-methyl-2-naphthaleneacetic acid
(*S*)-6-Methoxy-α-methyl-2-naphthaleneacetic acid
Laraflex
RN: 22204-53-1 **MP** (°C)**:** 155.3
MW: 230.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-05	9.924E-03	5	F306	1 0 1 2 2	intrinsic
6.948E-05	1.600E-02	21	B331	1 2 2 1 2	pH 7.4
6.080E-05	1.400E-02	25	A408	2 0 1 2 0	int
6.905E-05	1.590E-02	25	A427	0 0 0 0 0	
6.905E-05	1.590E-02	25	C059	1 2 1 1 2	
6.900E-05	1.589E-02	25	F306	1 0 1 2 2	intrinsic
1.146E-04	2.639E-02	37	F306	1 0 1 2 2	intrinsic
2.171E-05	5.000E-03	37	Y421	0 0 0 0 0	
5.211E-04	1.200E-01	amb	L434	0 0 0 0 0	
5.646E-05	1.300E-02	rt	H302	0 0 2 1 2	intrinsic

3276. $C_{14}H_{14}O_3S$

o-Cresyl-*p*-toluene sulfonate
2-Methylphenyl tosylate
o-Tolyl tosylate
2-Tolyl tosylate
RN: 599-75-7 **MP** (°C)**:**
MW: 262.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.144E-04	3.000E-02	ns	F014	0 0 0 0 0	

3277. $C_{14}H_{14}O_4$

Diallyl *m*-phthalate

RN: **MP** (°C)**:**
MW: 246.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-04	4.900E-02	25	S417	0 0 0 0 0	

3278. $C_{14}H_{14}O_4$

Diallyl phthalate
Di-2-propenyl phthalate

RN: 131-17-9 **MP** (°C)**:** –70
MW: 246.27 **BP** (°C)**:** 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.06E-04	<10.00E-02	20	F070	1 0 0 0 1	
7.390E-04	1.820E-01	20	L300	2 1 0 2 2	
7.413E-04	1.826E-01	ns	S460	0 0 0 0 0	

3279. $C_{14}H_{15}N$

p-Aminostilbene
4-Aminostilbene

RN: 834-24-2 **MP** (°C)**:**
MW: 197.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	5.000E-03	rt	N015	0 0 2 2 0	

3280. $C_{14}H_{15}NO_5$

L-Proline, 1-[(benzoyloxy)acetyl]-

RN: 115178-75-1 **MP** (°C)**:** 72.5
MW: 277.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-02	7.100E+00	22	N317	1 1 2 1 2	

3281. $C_{14}H_{15}N_3$

o-Aminoazotoluene
2-Amino-5-azotoluene

RN: 97-56-3 **MP** (°C)**:** 101
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.107E-05	7.000E-03	37	H120	1 1 1 1 1	normal saline

3282. $C_{14}H_{15}N_3$

p-Dimethylaminoazobenzene
4-Dimethylaminoazobenzol
Dimethylaminoazobenzene
Methylgelb
C. I. Solvent yellow 2

RN: 60-11-7 **MP** (°C)**:** 116
MW: 225.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.877E-04	2.000E-01	20	F300	1 0 0 0 0	
6.214E-06	1.400E-03	20	J027	1 0 0 0 1	
1.700E-06	3.830E-04	25	B333	0 0 0 0 0	*sic*
1.775E-06	4.000E-04	30	R430	0 0 0 0 0	
7.101E-04	1.600E-01	rt	D021	0 0 1 1 1	*sic*

3283. $C_{14}H_{15}N_3O_3S$

Gly-dapsone
Acetamide, 2-amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]

RN: 160349-02-0 **MP** (°C)**:**
MW: 305.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.849E-03	8.700E-01	25	P351	0 0 0 0 0	pH 7.4
>4.91E-02	>1.50E+01	25	P351	0 0 0 0 0	

3284. $C_{14}H_{15}N_5O_5$

9-(2-*O*-Butyryl-β-D-arabinofuranosyl)adenine
9H-Purin-6-amine, 9-[3,5-*bis*-*O*-[(1,1-dimethylethyl)dimethylsilyl]-2-*O*-(1-oxobutyl)-β-D-arabinofuranosyl]-

RN: 87970-05-6 **MP** (°C)**:**
MW: 333.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-04	3.410E-02	37	B306	1 2 0 1 2	pH 7.3

3285. $C_{14}H_{15}N_5O_6S$

Metasulfron-methyl
Metsulfuron methyl ester
Allie
Escort
DPX-T6376
Ally

RN: 74223-64-6 **MP** (°C)**:** 158
MW: 381.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-05	2.700E-02	ns	R427	0 0 0 0 0	

3286. $C_{14}H_{15}O_2PS_2$

Edifenphos

RN: 17109-49-8 **MP** (°C)**:**
MW: 310.38 **BP** (°C)**:** 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.803E-04	5.596E-02	ns	S460	0 0 0 0 0	

3287. $C_{14}H_{16}ClN_3O_2$

Triadimefon

1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone

Triamefon

Bayleton

RN: 43121-43-3 **MP** (°C)**:** 82.3
MW: 293.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.851E-04	2.600E-01	20	M161	1 0 0 0 2	

3288. $C_{14}H_{16}ClO_5PS$

Coumaphos

O,O-Diethyl *O*-(3-chloro-4-methylcoumarinyl-7) thiophosphate

RN: 56-72-4 **MP** (°C)**:** 91
MW: 362.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.135E-06	1.500E-03	20	M061	1 0 0 0 1	
4.169E-06	1.512E-03	ns	R427	0 0 0 0 0	

3289. $C_{14}H_{16}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid cyclohexyl ester

Cyclohexyl 2,4-dichlorophenoxyacetate

RN: 65267-97-2 **MP** (°C)**:**
MW: 303.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.811E-05	5.492E-03	ns	M120	0 0 1 1 2	

3290. $C_{14}H_{16}FN_3O_3$

2,5-Diaziridinyl-3-floro-6-morpholino-1,4-benzoquinone

2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1-aziridinyl)-3-fluoro-6-(4-morpholinyl)-

RN: 59886-45-2 **MP** (°C)**:** 157
MW: 293.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-03	2.000E+00	rt	C317	0 0 0 0 0	

3291. $C_{14}H_{16}F_3N_3O_4$

Profluralin
N-(Cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine
Pregard
Tolban
ER-5461

RN: 26399-36-0 **MP** (°C)**:** 32
MW: 347.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E-07	1.000E-04	20	E048	1 2 1 1 0	
2.879E-07	1.000E-04	20	M161	1 0 0 0 0	
2.879E-07	1.000E-04	27	K315	1 0 0 0 1	

3292. $C_{14}H_{16}N_2$

o-Tolidine
3,3′-Dimethylbenzidine

RN: 119-93-7 **MP** (°C)**:** 130.0
MW: 212.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E-03	1.300E+00	25	B068	2 0 1 1 1	

3293. $C_{14}H_{16}N_2O_2$

3,3′-Dimethoxybenzidine
o-Dianisidine
Dianisidine

RN: 119-90-4 **MP** (°C)**:** 137
MW: 244.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.456E-04	6.000E-02	25	B068	2 0 1 1 0	

3294. $C_{14}H_{16}N_2O_4$

2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-

RN: 116482-82-7 **MP** (°C)**:** 194.5
MW: 276.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	N317	1 1 2 1 2	

3295. $C_{14}H_{16}N_2O_4$
2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-
RN: 106231-69-0 **MP** (°C)**:**
MW: 276.29 **BP** (°C)**:** 570.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	B427	1 0 0 1 1	

3296. $C_{14}H_{16}N_2O_4S_2$
4-Thiazolidinecarboxylic acid, 2,2′-(1,4-phenylene)*bis*-
4-Thiazolidinecarboxylic acid, 2,2′-*p*-phenylenebis-
RN: 83690-84-0 **MP** (°C)**:**
MW: 340.42 **BP** (°C)**:** 697.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	6.128E-01	21	B414	1 0 0 1 1	fast decomposition

3297. $C_{14}H_{16}N_4$
Disperse black 3
N,N-Dimethyl-4,4′-azodian
4-Amino-4′-(dimethylamino)azobenzene
C.I. 11025
RN: 539-17-3 **MP** (°C)**:**
MW: 240.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	1.202E-04	25	B333	0 0 0 0 0	

3298. $C_{14}H_{16}N_4O_2S$
2-Sulfanilamido-5,6,7,8-tetrahydroquinazoline
2-Sulfanilamido-5,6,7,8,-tetrahydroquinazoline
RN: 71119-34-1 **MP** (°C)**:** 255
MW: 304.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-04	6.800E-02	29	C049	0 0 0 0 0	

3299. $C_{14}H_{16}N_4O_3S$
*N*4-Acetylsulfamethazine
*N*4-Acetylsulfamezathine
*N*4-Acetylsulphamethazine
Acetylsulfamethazine
2-*p*-Acetamidobenzenesulphonamido-4:6-dimethylpyri-
RN: 100-90-3 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-03	9.291E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
3.590E-03	1.150E+00	37	L091	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	M057	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	R075	1 2 0 0 2	
2.197E-03	7.040E-01	37	S192	1 0 1 1 2	pH 6.0
2.622E-03	8.400E-01	38	K006	1 0 0 0 1	

3300. $C_{14}H_{16}N_4O_3S$
*N*4-Acetylsulphasomidine
Acetamide, *N*-[4-[[(2,6-dimethyl-4-pyrimidinyl)amino]sulfonyl]phenyl]-
RN: 3163-31-3 **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.373E-04	4.400E-02	ns	B133	0 2 0 0 1	pH 7.4

3301. $C_{14}H_{16}N_4O_3S$
2-(*N*4-Acetylsulfanilylamino)-4-ethylpyrimidine
RN: **MP** (°C)**:**
MW: 320.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.435E-05	7.800E-03	37	R076	1 2 0 0 2	

3302. $C_{14}H_{16}N_4O_4S$
*N*4-Acetylsulphamethomidine
RN: **MP** (°C)**:**
MW: 336.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.730E-04	2.600E-01	ns	B133	0 2 0 0 2	pH 7.4

3303. $C_{14}H_{16}N_4O_5S$

*N*4-Acetylsulphadimethoxine
*N*4-Acetyl-2,4-dimethoxy-6-sulfanilamidopyrimidine
*N*4-Acetylsulfadimethoxypyrimidine
Sulfadimethoxine *N*4-acetate
RN: 555-25-9 **MP** (°C)**:**
MW: 352.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.392E-04	1.900E-01	ns	B133	0 2 0 0 2	pH 7.4

3304. $C_{14}H_{16}O_6$

Benzoic acid, 2-(acetyloxy)-, (1-oxobutoxy)methyl ester
RN: 118247-07-7 **MP** (°C)**:** 0il
MW: 280.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.249E-03	3.500E-01	21	N335	0 0 0 0 0	

3305. $C_{14}H_{16}O_6$

Ethylphthalyl ethyl glycolate
Ethoxycarbonylmethyl ethyl phthalate
Ethylphthalyl ethylglycolate
RN: 84-72-0 **MP** (°C)**:** 20
MW: 280.28 **BP** (°C)**:** 320

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-03	<7.99E-01	20	F070	1 0 0 0 1	

3306. $C_{14}H_{17}ClNO_4PS_2$

Dialifos
Dialifor
Diethyl *S*-(2-chloro-1-phthalimidoethyl) phosphorodithioate
Torak
Hercules 14503
RN: 10311-84-9 **MP** (°C)**:** 67
MW: 393.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.570E-07	1.800E-04	ns	F071	0 1 2 1 1	
4.571E-07	1.800E-04	ns	R427	0 0 0 0 0	

3307. $C_{14}H_{17}NO$
1-Cinnamoylpiperidine
N,N-Pentamethylenecinnamamide
1-(1-Oxo-3-phenyl-2-propenyl)-piperidine
RN: 5422-81-1 **MP** (°C)**:**
MW: 215.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	2.067E-01	ns	H350	0 0 0 0 0	

3308. $C_{14}H_{17}NO$
N-Cyclopentylcinnamamide
2-Propenamide, *N*-cyclopentyl-3-phenyl-
RN: 59831-97-9 **MP** (°C)**:**
MW: 215.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.280E-04	4.909E-02	ns	H350	0 0 0 0 0	

3309. $C_{14}H_{17}NO_2S$
m-Carboxylhexylphenylisothiocyanate
3-Carboxylhexylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 263.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.844E-02	25	K032	2 2 0 1 1	

3310. $C_{14}H_{17}NO_3$
Piperidine, 1-[(benzoyloxy)acetyl]-
RN: 106231-67-8 **MP** (°C)**:** 88
MW: 247.30 **BP** (°C)**:** 433.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.154E-03	7.800E-01	22	B427	1 0 0 1 1	
3.154E-03	7.800E-01	22	N317	1 1 2 1 2	

3311. $C_{14}H_{17}NO_4$
4-Piperidinol, 1-[(benzoyloxy)acetyl]-
RN: 115178-71-7 **MP** (°C)**:** 121.5
MW: 263.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.482E-02	1.180E+01	22	N317	1 1 2 1 2	

3312. $C_{14}H_{17}NO_5$

Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-, ethyl ester

RN: 106231-63-4 **MP** (°C)**:** 39.5
MW: 279.30 **BP** (°C)**:** 426.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-02	6.000E+00	22	B427	1 0 0 1 1	in 0.01M HCl
2.148E-02	6.000E+00	22	N317	1 1 2 1 2	

3313. $C_{14}H_{17}N_5O_3$

Pipemidic acid
Pipemidique acide

RN: 51940-44-4 **MP** (°C)**:** 253
MW: 303.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-03	3.215E-01	25	D051	2 0 0 1 2	0.05N NaCl
1.160E-03	3.519E-01	37	D051	2 0 0 1 2	0.05N NaCl

3314. $C_{14}H_{18}ClN_3S$

Chlorothen
N,N-Dimethyl-*N′*-(2-pyridyl)-*N′*-(5-chloro-2-thenyl)ethylenediamine
Chloromethapyrilene
5-Chloro-*N*-(2-(dimethylamino)ethyl)-*N*-(2-pyridyl)-2-thenylamine
Chloropyrilene

RN: 148-65-2 **MP** (°C)**:**
MW: 295.84 **BP** (°C)**:** 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	2.012E+00	37.5	L034	2 2 0 1 2	pH 7.4

3315. $C_{14}H_{18}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *n*-hexyl ester
Chloroxone
Agrotect
Amoxone
BH 2,4-D

RN: 1917-95-9 **MP** (°C)**:**
MW: 305.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.941E-05	5.924E-03	ns	M120	0 0 1 1 2	

3316. $C_{14}H_{18}N_2O$

Propyphenazone
Isopropylantipyrine
1,2-Dihydro-1,5-dimethyl-4-(isopropyl)-2-phenyl-pyrazol-3-one
4-Isopropyl-2,3-dimethyl-5-oxo-1-phenyl-3-pyrazoline
RN: 479-92-5 **MP** (°C)**:** 103
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.383E+00	7.791E+02	4.62	M109	2 1 1 1 0	EFG
3.330E+00	7.670E+02	10.93	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	15.02	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	20.96	M109	2 1 1 1 0	EFG
3.229E+00	7.436E+02	25.35	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	29.87	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	38.37	M109	2 1 1 1 0	EFG
3.348E+00	7.711E+02	40.32	M109	2 1 1 1 0	EFG

3317. $C_{14}H_{18}N_2O_3$

Reposal
5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetri-one
5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethylbarbituric acid
RN: 3625-25-0 **MP** (°C)**:** 213
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-03	4.407E-01	25	V033	2 0 1 1 2	
1.700E-03	4.459E-01	25.00	T303	1 0 0 0 1	
2.300E-03	6.033E-01	35.00	T303	1 0 0 0 1	
2.500E-03	6.558E-01	45.00	T303	1 0 0 0 1	

3318. $C_{14}H_{18}N_2O_3$

Piperazine, 1-[(benzoyloxy)acetyl]-4-methyl-
RN: 106231-70-3 **MP** (°C)**:**
MW: 262.31 **BP** (°C)**:** 438.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>7.62E-01	>2.00E+02	22	B427	1 0 0 1 1	

3319. $C_{14}H_{18}N_4O_2S$

2-Sulfanilylamino-4-isobutylpyrimidine
RN: 106596-34-3 **MP** (°C)**:**
MW: 306.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.264E-04	1.000E-01	37	R076	1 2 0 0 1	

3320. $C_{14}H_{18}N_4O_3$

Benomyl
(1-(Butylamino)carbonyl)-1H-benzimidazol-2-yl)carbamic acid methyl ester
RN: 17804-35-2 **MP** (°C)**:**
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	3.800E-03	20	A064	1 0 1 1 1	
1.309E-05	3.800E-03	20	M161	1 0 0 0 1	pH 7
~6.89E-06	~2.00E-03	ns	B309	0 0 0 0 0	

3321. $C_{14}H_{18}N_4O_3$

Trimethoprim
5-(3,4,5-Trimethoxybenzyl)-2,4-diaminopyrimidine
Monotrim
Syraprim
Proloprim
Trimpex
RN: 738-70-5 **MP** (°C)**:** 201
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	1.752E-02	22.5	B440	0 0 0 0 0	
1.396E-03	4.053E-01	25	H434	0 0 0 0 0	
1.378E-03	4.000E-01	25	M167	1 0 0 0 0	
1.722E-03	5.000E-01	32	D308	0 0 0 0 0	pH 8.54
2.711E-03	7.870E-01	37	G086	1 0 0 0 1	
1.378E-03	4.000E-01	37	M321	1 0 0 0 2	intrinsic
>1.72E-03	>5.00E-01	ns	B404	0 2 1 1 0	
1.378E-03	4.000E-01	ns	K444	0 0 0 0 0	

3322. $C_{14}H_{18}N_4O_6.0.5H_2O$

2′-Propionyl-6-methoxypurine arabinoside (hemihydrate)
RN: 145913-38-8 **MP** (°C)**:** 60–65
MW: 347.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-01	3.821E+01	37	C348	0 0 0 0 0	pH 7.00

3323. $C_{14}H_{18}N_4O_7.0.5H_2O$

9-[5-*O*-(Methoxyacetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 121032-38-0 **MP** (°C)**:** 137–139
MW: 363.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-02	2.838E+01	37	M378	1 2 1 1 2	pH 7.2

3324. $C_{14}H_{18}N_4O_7.0.9H_2O$

2′-Methoxyacetyl-6-methoxypurine arabinoside (0.9 hydrate)

RN: 145913-47-9 **MP** (°C)**:**
MW: 370.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.090E-02	3.368E+01	37	C348	0 0 0 0 0	pH 7.00

3325. $C_{14}H_{18}N_6O$

(1S,4R)-4-[2-Amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol sulfate (salt)

ABC sulfate[47]

ABC[48]

Abacavir

RN: 188062-50-2 **MP** (°C)**:**
MW: 286.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.867E-09	1.680E-06	32	M458	0 0 0 0 0	

3326. $C_{14}H_{18}N_6O_4$

2,5-Diaziridinyl-3,6-bis(glycinamide)-1,4-benzoquinone

RN: 59886-49-6 **MP** (°C)**:** 200
MW: 334.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.495E-03	5.000E-01	rt	C317	0 0 0 0 0	

3327. $C_{14}H_{18}O_4$

Diisopropyl phthalate

bis(1-Methyl-ethyl) phthalate

RN: 605-45-8 **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-03	3.329E-01	20	L300	2 1 0 2 2	

3328. $C_{14}H_{18}O_4$
Di-*n*-propyl phthalate
Dipropyl phthalate
RN: 131-16-8 **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-04	1.081E-01	20	L300	2 1 0 2 2	

3329. $C_{14}H_{18}O_4$
Diisopropyl *o*-phthalate
RN: **MP** (°C)**:**
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-04	1.670E-01	25	S417	0 0 0 0 0	

3330. $C_{14}H_{18}O_6$
Methyl glycol phthalate
bis(2-Methoxyethyl) phthalate
RN: 117-82-8 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-02	8.723E+00	15	H069	1 0 1 1 1	

3331. $C_{14}H_{18}O_6$
Ethyl phthalyl ethyl glycollate
RN: **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-03	4.998E-01	15	H069	1 0 1 1 0	
1.770E-03	4.998E-01	ns	F014	0 0 0 0 1	

3332. $C_{14}H_{18}O_6$
Dimethoxyethyl phthalate
1,2-Benzenedicarboxylic acid, di(2-methoxyethyl) ester
RN: 34006-76-3 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.986E-02	8.428E+00	20	F070	1 0 0 0 1	
2.944E-02	8.310E+00	ns	F014	0 0 0 0 2	

3333. $C_{14}H_{19}Cl_2NO_2$

Chlorambucil
N,N-di-(2-Chloroethyl)-γ-(*p*-aminophenyl)butyric acid
Linfolysin
Elcoril
Linfolizin
Leukersan

RN: 305-03-3 **MP** (°C)**:** 64
MW: 304.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	9.127E-02	3	G434	0 0 0 0 0	pH 4.13
<3.29E-03	<1.00E+00	30	L343	2 1 1 1 0	EFG

3334. $C_{14}H_{19}IN_2O_6$

Uridine, 2′-deoxy-5-iodo-, 5′-pentanoate
5′-Valeryl 5-iodo-2′-deoxyuridine

RN: 84052-69-7 **MP** (°C)**:** 142.5
MW: 438.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E+02	1.753E+05	25	N332	0 0 0 0 0	pH 7.4

3335. $C_{14}H_{19}IN_2O_6$

Uridine, 2′-deoxy-5-iodo-, 5′-(2,2-dimethylpropanoate)
5′-Pivaloyl 5-iodo-2′-deoxyuridine
5-Iodo-2′-deoxyuridine 5′-pivalate

RN: 84043-28-7 **MP** (°C)**:** 106.5
MW: 438.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E+02	1.928E+05	25	N332	0 0 0 0 0	pH 7.4

3336. $C_{14}H_{19}NO$

n-Pentylcinnamamide
2-Propenamide, *N*-pentyl-3-phenyl-

RN: 23784-51-2 **MP** (°C)**:**
MW: 217.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.782E-02	ns	H350	0 0 0 0 0	

3337. $C_{14}H_{19}NO_3$
Acetaminophen hexanoate
Hexanyl acetaminophen
Hexanoic acid, 4-(acetylamino)phenyl ester
4′-Hydroxyacetanilide hexanoate
RN: 20675-21-2 **MP** (°C)**:** 107
MW: 249.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.220E-05	1.800E-02	25	B010	1 1 1 1 0	
2.286E-04	5.700E-02	37	D029	0 0 0 0 0	

3338. $C_{14}H_{19}NO_3$
Propanamide, 2-(benzoyloxy)-*N*,*N*-diethyl-
RN: 115178-79-5 **MP** (°C)**:** 53.5
MW: 249.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.214E-03	1.300E+00	22	N317	1 1 2 1 2	

3339. $C_{14}H_{19}NO_4$
Anisomycin
(2R,3R,4R)-2-(4-Methoxybenzyl)-3,4-pyrrolidinediol-3-acetate
RN: 22862-76-6 **MP** (°C)**:** 140.5
MW: 265.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	6.550E+00	28	A038	2 0 1 1 2	

3340. $C_{14}H_{19}N_3S$
Methapyrilene
N,*N*-Dimethyl-*N*′,2-pyridinyl-*N*′-(2-thienylmethyl)-1,2-ethanediamine
Cope
A 3322
AH-42
Semiken
RN: 91-80-5 **MP** (°C)**:** <25
MW: 261.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	6.012E-01	30	L068	1 0 0 1 0	EFG
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3341. $C_{14}H_{19}N_3S$

Thenyldiamine
1,2-Ethanediamine, *N,N*-dimethyl-*N′*-2-pyridinyl-*N′*-(3-thienylmethyl)-
N-(2-Dimethylaminoethyl)-*N*-2-pyridyl-3-thenylamine
Thefanil
Thenfadil
Tenfidil

RN: 91-79-2 **MP** (°C)**:**
MW: 261.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3342. $C_{14}H_{19}N_5O_4$

N,N-Diethylsuccinamyloxymethyl-1-allopurinol
Butanoic acid, 4-(diethylamino)-4-oxo-, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl) methyl ester

RN: 98827-27-1 **MP** (°C)**:** 138-140
MW: 321.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.027E-01	3.300E+01	22	B322	0 0 0 0 0	

3343. $C_{14}H_{19}N_5O_5$

9-[5′-(*O*-Butyryl)-β-D-arabinofuranosyl]adenine ester
Vidarabine 5′-butyrate

RN: 65926-30-9 **MP** (°C)**:**
MW: 337.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-02	1.610E+01	ns	B134	0 1 1 1 2	

3344. $C_{14}H_{19}O_6P$

Crotoxyphos
Dimethylphosphate of α-methylbenzyl-3-hydroxy-*cis*-crotonate

RN: 7700-17-6 **MP** (°C)**:**
MW: 314.28 **BP** (°C)**:** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.179E-03	9.990E-01	ns	M061	0 0 0 0 0	
3.182E-03	1.000E+00	rt	M161	0 0 0 0 0	

3345. $C_{14}H_{20}ClNO_2$

Alachlor
2-Chloro-2′,6′-diethyl-*N*-(methoxymethyl)acetanilide
RN: 15972-60-8 **MP** (°C)**:** 39.5
MW: 269.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-04	2.400E-01	23	M161	1 0 0 0 2	
5.486E-04	1.480E-01	25	B200	1 0 0 0 2	
5.486E-04	1.480E-01	ns	M061	0 0 0 0 2	
5.560E-04	1.500E-01	ns	M110	0 0 0 0 0	EFG
8.896E-04	2.400E-01	ns	V414	0 0 0 0 0	

3346. $C_{14}H_{20}ClNO_2$

Acetochlor
Doubleplay
Harness
Topnotch
Top Hand
Acenit
RN: 34256-82-1 **MP** (°C)**:**
MW: 269.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.260E-04	2.228E-01	ns	S460	0 0 0 0 0	

3347. $C_{14}H_{20}N_2O$

Siduron
1-(2-Methylcyclohexyl)-3-phenylurea
RN: 1982-49-6 **MP** (°C)**:** 133
MW: 232.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.748E-05	1.800E-02	25	B200	1 0 0 0 1	
7.748E-05	1.800E-02	25	G036	1 0 0 0 1	
7.748E-05	1.800E-02	25	M161	1 0 0 0 1	

3348. $C_{14}H_{20}N_2O_2$
Pindolol
Barbloc
Visken
2-Propanol, 1-(1H-indol-4-yloxy)-3-[(-methylethyl)amino]-
RN: 13523-86-9 **MP** (°C)**:**
MW: 248.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-04	3.300E-02	22.5	B422	2 0 2 2 2	

3349. $C_{14}H_{20}N_2O_3S$
Tolcyclamide
1-Cyclohexyl-3-*para*-tolylsulfonylurea
Glycyclamide
RN: 664-95-9 **MP** (°C)**:** 175
MW: 296.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.194E-05	1.836E-02	37	A028	1 0 2 1 2	intrinsic
6.200E-05	1.838E-02	37	A046	2 0 1 1 2	

3350. $C_{14}H_{20}N_3O_5PS$
Pyrazophos
2-[(Diethoxyphosphinothioyl)oxy]-5-methylpyrazolo[1,5-a]pyrimidine-6-carboxylic acid ethyl Ester
Afugan
Curamil
RN: 13457-18-6 **MP** (°C)**:** 50.5
MW: 373.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.125E-05	4.200E-03	20	A306	0 0 0 0 0	
1.125E-05	4.200E-03	20	M161	1 0 0 0 1	

3351. $C_{14}H_{20}N_4O_2$
2,5-bis(Methylaziridinyl)-3,6-bis(methylamino)-1,4-benzoquinone
RN: 64947-06-4 **MP** (°C)**:** 179
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.62E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3352. $C_{14}H_{20}N_4O_2$

2,5-Diaziridinyl-3,6-bis(dimethylamino)-1,4-benzoquinone

RN: 59886-50-9 **MP** (°C)**:** 112
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-02	1.000E+01	rt	C317	0 0 0 0 0	

3353. $C_{14}H_{20}N_4O_2$

2,5-Diaziridinyl-3,6-bis(ethylamino)-1,4-benzoquinone

RN: 59886-53-2 **MP** (°C)**:** 157
MW: 276.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.809E-03	5.000E-01	rt	C317	0 0 0 0 0	

3354. $C_{14}H_{20}N_4O_4$

2,5-Diaziridinyl-3,6-bis(hydroxyethylamino)-1,4-benzoquinone

RN: 59886-54-3 **MP** (°C)**:** 188
MW: 308.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-03	2.000E+00	rt	C317	0 0 0 0 0	

3355. $C_{14}H_{20}O_3$

Heptyl *p*-hydroxybenzoate
n-Heptyl 4-hydroxybenzoate

RN: 1085-12-7 **MP** (°C)**:** 48
MW: 236.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	6.215E-02	–244	B355	0 0 0 0 0	
2.010E-04	4.750E-02	15	B355	0 0 0 0 0	
2.520E-04	5.955E-02	20	B355	0 0 0 0 0	
5.827E-03	1.377E+00	25	D081	1 2 2 1 2	*sic*
1.259E-04	2.975E-02	25	F322	2 0 1 1 0	EFG

3356. $C_{14}H_{21}NO_2$
Heptyl *p*-aminobenzoate
Heptyl 4-aminobenzoate
RN: 14309-40-1 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	4.707E-03	37	F006	1 1 2 2 1	
3.300E-05	7.766E-03	ns	M066	0 0 0 0 1	

3357. $C_{14}H_{21}NO_2$
2,6-Diisopropyl-4-acetaminophenol
3,5-Diisopropylparacetamol
4-Acetamido-2,6-diisopropylphenol
RN: 1988-14-3 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.844E-04	1.375E-01	25	D078	1 2 2 1 2	

3358. $C_{14}H_{21}NO_2$
Octyl nicotinate
Nicotinic acid *n*-octyl ester
RN: 70136-02-6 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.249E-05	1.000E-02	32	L346	1 0 0 1 2	

3359. $C_{14}H_{21}NO_2$
Benzeneacetamide, *N*-hydroxy-α-dipropyl
RN: 60631-09-6 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	3.059E-01	26	G076	1 0 0 0 1	

3360. $C_{14}H_{21}NO_2$
Benzenepropanamide, *N*-hydroxy-α2,4,6-pentamethyl
RN: 60631-10-9 **MP** (°C)**:**
MW: 235.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.060E-02	26	G076	1 0 0 0 1	

3361. $C_{14}H_{21}NO_3$

4-Methoxybenzoic acid-2-(diethylamino)ethyl ester
Diethylaminoethyl *p*-anisate
RN: 10367-84-7 **MP** (°C)**:**
MW: 251.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.332E+00	ns	M066	0 0 0 0 1	

3362. $C_{14}H_{21}NO_4P$

Phenyl(di-morpholido)-phosphate
RN: **MP** (°C)**:**
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	7.706E+02	25	A040	1 0 0 0 2	

3363. $C_{14}H_{21}N_3O_3$

Karbutilate
m-(3,3-Dimethylureido)phenyl-*tert*-butylcarbamate
Tandex
RN: 4849-32-5 **MP** (°C)**:** 176.3
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-03	3.250E-01	20	B200	1 0 0 0 2	
1.163E-03	3.250E-01	rt	M161	0 0 0 0 2	

3364. $C_{14}H_{21}N_3O_3S$

Tolazamide
N-(((Hexahydro-1H-azepin-1-yl)amino)carbonyl)-4-methylbenzenesulfonamide
Tolinase
N-(*p*-Toluenesulfonyl)-*N′*-hexamethyleniminourea
U 17835
RN: 1156-19-0 **MP** (°C)**:** 170
MW: 311.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.540E-02	30	H025	1 0 2 1 1	intrinsic
1.124E-03	3.499E-01	ns	B404	0 2 1 1 0	

3365. $C_{14}H_{22}$

2-Octylbenzene
(1-Methylheptyl)benzene
RN: 777-22-0 **MP** (°C)**:**
MW: 190.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-06	3.017E-04	ns	D001	0 0 0 0 2	

3366. $C_{14}H_{22}N_2O$

Lidocaine
2-(Diethylamino)-*N*-(2,6-dimethylphenyl)acetamide
2-Diethylamino-2′,6′-acetoxylidide
Lignocaine
Leostesin
Xylocaine
RN: 137-58-6 **MP** (°C)**:** 68
MW: 234.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-02	4.335E+00	14.5	N046	2 0 1 1 1	intrinsic
5.460E-05	1.279E-02	22.5	B440	0 0 0 0 0	
1.550E-02	3.632E+00	25	D402	1 2 2 2 0	EFG
1.643E-02	3.850E+00	25	L338	1 0 1 1 2	
1.630E-02	3.820E+00	25	N046	2 0 1 1 1	intrinsic
1.488E-02	3.488E+00	25	S450	0 0 0 0 0	Intrinsic
1.750E-02	4.101E+00	30	L068	1 0 0 1 0	EFG
1.460E-02	3.421E+00	34.5	N046	2 0 1 1 1	intrinsic
1.700E-02	3.984E+00	37	D402	1 2 2 2 0	
1.440E-02	3.375E+00	37	N044	2 1 1 2 2	intrinsic

3367. $C_{14}H_{22}N_2O_2$

4-Methylaminobenzoic acid-2-(diethyl-amino)ethyl ester
Benzoic acid, 4-(methylamino)-, 2-(diethylamino)ethyl ester
Benzoic acid, *p*-(methylamino)-, 2-(diethylamino)ethyl ester
RN: 16488-52-1 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-03	1.940E+00	ns	M066	0 0 0 0 2	

3368. $C_{14}H_{22}N_2O_2$
4-Aminobenzoic acid-2-(diethyl-amino)propyl ester
2-Diethylamino)propyl 4-aminobenzoate
RN: 5878-13-7 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.229E+00	ns	M066	0 0 0 0 2	

3369. $C_{14}H_{22}N_2O_3$
2,4-Diazaspiro[5.10]hexadecane-1,3,5-trione
RN: 143288-63-5 **MP** (°C)**:**
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	6.925E-03	25	P350	0 0 0 0 0	intrinsic

3370. $C_{14}H_{22}N_2O_3$
Atenolol
Anselol
Apo-atenolol
Benzeneacetamide
4-(2′-Hydroxy-3′-((1-methylethyl)amino)propoxy)-
Noten
RN: 29122-68-7 **MP** (°C)**:**
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.069E-05	1.350E-02	25	A408	2 0 1 2 0	int
7.134E-10	1.900E-07	32	M458	0 0 0 0 0	
9.950E-02	2.650E+01	ns	K444	0 0 0 0 0	

3371. $C_{14}H_{22}N_2O_4$
Ethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate
Ethyl 2-methyl-2-cyclohexenyl-6-methylmalonurate
RN: **MP** (°C)**:** 97.5
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.823E-01	23	B152	1 2 1 1 1	pH 3.5

3372. $C_{14}H_{22}N_2O_5$

Methoxymethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate

RN: **MP** (°C)**:** 73
MW: 298.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	1.134E+00	23	B152	1 2 1 1 1	pH 3.5

3373. $C_{14}H_{22}O$

Methyl ionone
6-Methylionone

RN: 1335-46-2 **MP** (°C)**:**
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.693E-05	2.000E-02	25	M350	1 0 1 1 1	

3374. $C_{14}H_{22}O$

o-*n*-Octylphenol
2-*n*-Octylphenol

RN: 949-13-3 **MP** (°C)**:**
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	2.857E-03	25	L022	1 0 0 0 0	

3375. $C_{14}H_{22}O$

p-*n*-Octylphenol
4-Octylphenol

RN: 1806-26-4 **MP** (°C)**:** 44.5
MW: 206.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.107E-05	1.260E-02	20.5	A335	0 0 0 0 0	
6.120E-05	1.263E-02	20.5	A335	0 0 0 0 0	
8.812E-06	1.818E-03	25	L022	1 0 0 0 0	

3376. $C_{14}H_{23}O_3P$

Dibutyl phenyl phosphonate
Dibutoxyphenylphosphine oxide
Dibutyl phenylphosphonate
RN: 1024-34-6 **MP** (°C)**:**
MW: 270.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.40E-04	<2.00E-01	25	B070	1 2 0 1 0	

3377. $C_{14}H_{24}NO_4PS_3$

Bensulide
O,O-bis(1-Methylethyl) *S*-(2-((phenylsulfonyl)amino)ethyl) phosphorodithioate
Betasan
Betamec
Exporsan
Benzulfide
RN: 741-58-2 **MP** (°C)**:** 34.4
MW: 397.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-05	2.500E-02	20	B200	1 2 0 0 1	
6.289E-05	2.500E-02	rt	M161	0 0 0 0 1	

3378. $C_{14}H_{24}N_2O_3$

5-Ethyl-5-*n*-octylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-octyl-
5-Ethyl-5-octylbarbiturate
RN: 64810-90-8 **MP** (°C)**:**
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	3.059E-02	25	M310	2 2 2 2 2	

3379. $C_{14}H_{24}N_2O_3$

p-5-Ethyl-5-methylhexylcarbinylbarbituric acid
RN: **MP** (°C)**:**
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-03	4.140E-01	ns	T003	0 0 0 0 2	

3380. $C_{14}H_{24}O_2$

3-Hydroxy-2,5-dispirocyclohexyltetrahydrofuran
7-Oxadispiro[5.1.5.2]pentadecan-14-ol
RN: 29839-63-2 **MP** (°C)**:**
MW: 224.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.098E-02	6.951E+00	rt	B066	0 2 0 0 0	contains impurity

3381. $C_{14}H_{26}O_4$

1,12-Dodecanedicarboxylic acid
Tetradecanedioic acid
RN: 821-38-5 **MP** (°C)**:** 127
MW: 258.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.741E-04	2.000E-01	21	B040	1 0 1 1 0	*sic*

3382. $C_{14}H_{27}NO_2$

Pentanamide,*N*-hydroxy-α,α-dipropyl
RN: **MP** (°C)**:**
MW: 241.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.207E-01	26	G076	1 0 0 0 1	

3383. $C_{14}H_{28}NO_3PS_2$

Piperophos
S-(2-(2-Methyl-1-piperidinyl)-2-oxoethyl) *O,O*-dipropyl phosphorodithioate
RN: 24151-93-7 **MP** (°C)**:**
MW: 353.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.072E-05	2.500E-02	20	M161	1 0 0 0 1	

3384. $C_{14}H_{28}N_2O_2$

N,N,N′,N′-Tetramethylsebacamide
Decanediamide, *N,N,N′,N′*-tetramethyl-
RN: 13424-83-4 **MP** (°C)**:**
MW: 256.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.270E-01	1.351E+02	30	D010	1 2 1 1 2	

3385. $C_{14}H_{28}O_2$

Myristic acid
Tetradecanoic acid
Crodacid
1-Tridecanecarboxylic acid

RN: 544-63-8 **MP** (°C)**:** 54
MW: 228.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.692E-05	1.300E-02	0	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	D041	1 0 0 0 0	
8.757E-05	2.000E-02	20	R001	1 1 1 1 1	
4.700E-06	1.073E-03	25	J001	1 0 2 1 1	average of 2
8.000E-07	1.827E-04	25	R002	0 0 0 0 0	intrinsic
3.710E-06	8.473E-04	25	R002	0 0 0 0 0	
9.633E-05	2.200E-02	30	B136	1 0 2 1 1	
1.051E-04	2.400E-02	30	R001	1 1 1 1 1	
1.270E-04	2.900E-02	40	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	R001	1 1 1 1 1	
1.839E-05	4.200E-03	50	E005	2 1 1 2 1	
9.700E-06	2.215E-03	50	J001	1 0 2 1 1	
1.489E-04	3.400E-02	60	B136	1 0 2 1 1	
2.452E-05	5.600E-03	60	E005	2 1 1 2 1	
1.489E-04	3.400E-02	60	R001	1 1 1 1 1	
5.692E-05	1.300E-02	.0	R001	1 1 1 1 1	

3386. $C_{14}H_{28}O_4$

1,3-Dioxolane-4-methanol, 2-[2-(heptyloxy)ethyl]-2-methyl

RN: 143458-57-5 **MP** (°C)**:**
MW: 260.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.440E-03	1.156E+00	25	P342	0 0 0 0 0	0.0001M Na_2CO_3

3387. $C_{14}H_{29}NO_2$

Benzenepropanamide, *N*-hydroxy-α2,3-pentamethyl
Octanamide, *N*-hydroxy-2,2-dipropyl

RN: 60631-08-5 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	
1.500E-03	3.651E-01	26	G076	1 0 0 0 1	

3388. $C_{14}H_{29}NO_2$
Octanamide, 2,2,4-triethyl-*N*-hydroxy
RN: 60631-07-4 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	

3389. $C_{14}H_{29}NO_2$
Decanamide, 2,2-diethyl-*N*-hydroxy
RN: 60631-06-3 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.460E-03	26	G076	1 0 0 0 1	

3390. $C_{14}H_{29}NO_2$
Dodecanamide, *N*-hydroxy-2,2-dimethyl
RN: 60631-05-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.894E-03	26	G076	1 0 0 0 1	

3391. $C_{14}H_{29}NO_2$
Pentanamide, *N*-hydroxy-4-methyl-2,2-bis(2-methylpropyl)
RN: 60469-53-6 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+01	2.434E+03	26	G076	1 0 0 0 1	

3392. $C_{14}H_{29}NO_2$
Hexanamide, 2,2-dibutyl-*N*-hydroxy
2,2-Dibutyl-*N*-hydroxyhexanamide
Tri-*n*-butylacetohydroxamic acid
RN: 52061-82-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.704E-02	26	G076	1 0 0 0 1	

3393. $C_{14}H_{29}NO_2$

Tetradecanamide, *N*-hydroxy
Myristohydroxamic acid
N-Hydroxytetradecanamide
RN: 17698-03-2 **MP** (°C)**:**
MW: 243.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-04	2.434E-02	26	G076	1 0 0 0 1	

3394. $C_{14}H_{30}$

n-Tetradecane
Tetradecane
RN: 629-59-4 **MP** (°C)**:** 5.89
MW: 198.40 **BP** (°C)**:** 253.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.663E-09	3.300E-07	23	C332	0 0 0 0 0	
3.500E-08	6.944E-06	25	F004	0 0 0 0 0	
1.159E-08	2.300E-06	ns	H123	0 0 0 0 0	

3395. $C_{14}H_{30}O$

Tetradecanol
RN: 27196-00-5 **MP** (°C)**:**
MW: 214.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-06	3.130E-04	25	R002	0 0 0 0 0	

3396. $C_{14}H_{30}O$

Myristyl alcohol
Tetradecanol
RN: 112-72-1 **MP** (°C)**:** 38
MW: 214.39 **BP** (°C)**:** 289

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.049E-08	1.940E-05	4	H030	2 2 2 2 2	
9.049E-08	1.940E-05	4	H103	1 2 2 2 2	
8.909E-07	1.910E-04	25	H103	1 2 2 2 2	
5.737E-07	1.230E-04	32	H030	2 2 2 2 2	
5.737E-07	1.230E-04	32	H103	1 2 2 2 2	
1.105E-06	2.370E-04	45	H030	2 2 2 2 2	
1.105E-06	2.370E-04	45	H103	1 2 2 2 2	
2.094E-06	4.490E-04	61	H030	2 2 2 2 2	
2.094E-06	4.490E-04	61	H103	1 2 2 2 2	

3397. $C_{14}H_{31}O_2P$

Ethyl dihexyl phosphinate
Phosphinic acid, dihexyl-, ethyl ester
RN: 113977-19-8 **MP** (°C)**:**
MW: 262.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.81E-04	<1.00E-01	25	B070	1 2 0 1 0	

3398. $C_{14}H_{31}O_3P$

Dibutyl hexyl phosphonate
Phosphinic acid, hexyl-, dibutyl ester
RN: 5929-66-8 **MP** (°C)**:**
MW: 278.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.18E-04	<2.00E-01	25	B070	1 2 0 1 0	

3399. $C_{14}H_{31}O_3P$

Diethyl hexyl phosphonate
Phosphinic acid, hexyl-, diethyl ester
RN: 16165-66-5 **MP** (°C)**:**
MW: 278.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.155E-03	6.000E-01	25	B070	1 2 0 1 0	

3400. $C_{14}H_{31}O_4P$

Dibutyl hexyl phosphate
Phosphoric acid, dibutyl hexyl ester
RN: 80421-90-5 **MP** (°C)**:**
MW: 294.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3401. $C_{14}H_{31}O_4P$

Diethyl decyl phosphate
Phosphoric acid, decyl ester
RN: 20195-16-8 **MP** (°C)**:**
MW: 294.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3402. $C_{14}H_{31}O_5P$
Dibutyl ethoxybutyl phosphate
RN: 100888-67-3 **MP** (°C)**:**
MW: 310.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	7.000E-01	25	B070	1 2 0 1 0	

3403. $C_{15}H_{10}$
4,5-Methylenephenanthrene
4H-Cyclopenta[def]phenanthrene
RN: 203-64-5 **MP** (°C)**:** 76
MW: 190.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.782E-06	1.100E-03	27	D003	1 0 0 1 1	

3404. $C_{15}H_{10}Cl_2N_2O_2$
Lorazepam
Alzapam
Ativan
Apo-lorazepam
7-Chloro-5-(*o*-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
RN: 846-49-1 **MP** (°C)**:** 167
MW: 321.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.681E-04	5.400E-02	ns	N315	0 2 2 1 2	pH 7.09

3405. $C_{15}H_{10}O_2$
9-Anthracenecarboxylic acid
Anthracene-9-carboxylic acid
RN: 723-62-6 **MP** (°C)**:** 214
MW: 222.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.824E-04	8.499E-02	24	H106	1 0 2 2 2	
3.825E-07	8.500E-05	ns	M349	0 2 1 1 2	

3406. $C_{15}H_{10}O_4S$
7-Methylthio-2-xanthonecarboxylic acid
RN: 40363-76-6 **MP** (°C)**:**
MW: 286.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.081E-07	2.600E-04	25	C059	1 2 1 1 1	

3407. $C_{15}H_{10}O_5S$
7-Methylsulfinyl-2-xanthonecarboxylic acid
RN: 40691-50-7 **MP** (°C)**:**
MW: 302.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.064E-06	2.740E-03	25	C059	1 2 1 1 2	

3408. $C_{15}H_{10}O_6$
Eriodictyol
5,7,3′,4′-Tetra-hydroxyflavon
RN: 552-58-9 **MP** (°C)**:** 257dec
MW: 286.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.445E-04	7.000E-02	20	F300	1 0 0 0 1	
6.987E-04	2.000E-01	100	F300	1 0 0 0 2	

3409. $C_{15}H_{10}O_7$
Morin
3,5,7,2′,4′,-Penta-hydroxyflavon
RN: 480-16-0 **MP** (°C)**:** 299.5
MW: 302.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.271E-04	2.500E-01	20	F300	1 0 0 0 1	
2.978E-03	9.000E-01	100	F300	1 0 0 0 0	

3410. $C_{15}H_{10}O_7$

Quarcetin
2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one
3,3′,4′,5,7-Pentahydroxyflavone
3′,4′,5,7-Tetrahydroxyflavon-3-ol
Xanthaurine
Meletin

RN: 117-39-5 **MP** (°C)**:** 316–317
MW: 302.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.985E-02	6.000E+00	ns	Z411	0 0 0 0 0	

3411. $C_{15}H_{10}O_7.H_2O$

Morin hydrate
4H-1-Benzopyran-4-one, 2-(2,4-dihydroxyphenyl)-3,5,7-trihydroxy-, monohydrate
Flavone, 2′,3,4′,5,7-pentahydroxy-, monohydrate
Morin monohydrate

RN: 6202-27-3 **MP** (°C)**:**
MW: 320.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-04	1.920E-01	ns	B404	0 2 1 1 0	

3412. $C_{15}H_{11}ClF_3NO_4$

Oxyfluorfen
Oxyfluorofen
Koltar
Goal
2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene
Goal 1.6E

RN: 42874-03-3 **MP** (°C)**:** 83–84
MW: 361.71 **BP** (°C)**:** >240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.236E-07	1.170E-04	ns	R427	0 0 0 0 0	

3413. $C_{15}H_{11}ClN_2O_2$

Oxazepam
Serax
7-Chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one
Apo-oxazepam
Abboxampam

RN: 604-75-1 **MP** (°C)**:** 205.5
MW: 286.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-05	2.000E-02	22	N319	0 0 0 0 0	
1.744E-04	5.000E-02	amb	L434	0 0 0 0 0	
7.673E-05	2.200E-02	c	B362	0 0 0 0 0	

3414. $C_{15}H_{11}ClO_3$

Chlorflurecol-methyl
Chlorflurenol
Methyl-2-chloro-9-hydroxyfluorene-9-carboxylate

RN: 2536-31-4 **MP** (°C)**:** 152
MW: 274.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.552E-05	1.800E-02	20	A308	1 0 0 0 1	
7.936E-05	2.180E-02	20	B200	1 0 0 0 2	
6.552E-05	1.800E-02	20	M161	1 0 0 0 1	

3415. $C_{15}H_{11}NO_2$

C.I. Disperse orange 11
1-Amino-2-methylanthraquinone
2-Methyl-1-anthraquinonylamine
Acetate fast orange R

RN: 82-28-0 **MP** (°C)**:** 208
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.322E-04	25	B333	0 0 0 0 0	

3416. $C_{15}H_{11}NO_2$

C.I. Disperse red 9
1-(Methylamino)-9,10-anthraquinone
Serilene fast pink BT
Smoke red M

RN: 82-38-2 **MP** (°C)**:** 161
MW: 237.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-07	7.355E-05	25	B333	0 0 0 0 0	

3417. $C_{15}H_{11}NO_3$

N-epoxymethyl-1,8-naphthamilide
ENA

RN: **MP** (°C)**:**
MW: 253.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.580E-05	1.160E-02	ns	D428	0 0 0 0 0	

3418. $C_{15}H_{11}N_3$

2,2′,6,2″-terpyridine
Terpyridine
Tripyridyl

RN: 1148-79-4 **MP** (°C)**:**
MW: 233.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.310E-03	1.472E+00	24.99	B444	0 0 0 0 0	

3419. $C_{15}H_{11}N_3O_3$

Nitrazepam
1,3-Dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one
Mogadon
Unisomnia

RN: 146-22-5 **MP** (°C)**:** 224
MW: 281.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	4.300E-02	30	O321	0 0 0 0 0	

3420. $C_{15}H_{12}$

1-Methylphenanthrene

RN: 832-69-9 **MP** (°C)**:** 118
MW: 192.26 **BP** (°C)**:** 358

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-07	9.520E-05	6.60	M063	2 1 2 2 2	
4.950E-07	9.517E-05	6.60	M082	1 1 1 2 2	
4.950E-07	9.517E-05	6.60	M151	2 1 2 2 2	
4.956E-06	9.529E-04	6.64	M183	1 2 1 1 2	
5.929E-07	1.140E-04	8.90	M063	2 1 2 2 2	
5.940E-07	1.142E-04	8.90	M082	1 1 1 2 2	
5.940E-07	1.142E-04	8.90	M151	2 1 2 2 2	
5.933E-07	1.141E-04	8.94	M183	1 2 1 1 2	
7.646E-07	1.470E-04	14.00	M063	2 1 2 2 2	
7.650E-07	1.471E-04	14.00	M082	1 1 1 2 2	
7.650E-07	1.471E-04	14.00	M151	2 1 2 2 2	
7.650E-07	1.471E-04	14.04	M183	1 2 1 1 2	
1.004E-06	1.930E-04	19.20	M063	2 1 2 2 2	
1.010E-06	1.942E-04	19.20	M082	1 1 1 2 2	
1.010E-06	1.942E-04	19.20	M151	2 1 2 2 2	
1.004E-06	1.931E-04	19.24	M183	1 2 1 1 2	
1.326E-06	2.550E-04	24.10	M063	2 1 2 2 2	
1.320E-06	2.538E-04	24.10	M082	1 1 1 2 2	
1.320E-06	2.538E-04	24.10	M151	2 1 2 2 2	
1.327E-06	2.552E-04	24.14	M183	1 2 1 1 2	
1.399E-06	2.690E-04	25.00	M151	2 1 1 2 2	
1.581E-06	3.040E-04	26.90	M063	2 1 2 2 2	
1.580E-06	3.038E-04	26.90	M082	1 1 1 2 2	
1.580E-06	3.038E-04	26.90	M151	2 1 2 2 2	
1.583E-06	3.043E-04	26.94	M183	1 2 1 1 2	
1.846E-06	3.550E-04	29.90	M063	2 1 2 2 2	
1.850E-06	3.557E-04	29.90	M082	1 1 1 2 2	
1.850E-06	3.557E-04	29.90	M151	2 1 2 2 2	
1.848E-06	3.553E-04	29.94	M183	1 2 1 1 2	

3421. $C_{15}H_{12}$

2-Methylanthracene

RN: 613-12-7 **MP** (°C)**:** 204
MW: 192.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-08	7.060E-06	6.30	M063	2 1 2 2 2	
3.670E-08	7.056E-06	6.30	M082	1 1 1 2 2	
3.670E-08	7.056E-06	6.30	M151	2 1 2 2 2	
3.675E-08	7.066E-06	6.34	M183	1 2 1 1 2	
4.411E-08	8.480E-06	9.10	M063	2 1 2 2 2	
4.410E-08	8.479E-06	9.10	M082	1 1 1 2 2	
4.410E-08	8.479E-06	9.10	M151	2 1 2 2 2	
4.414E-08	8.487E-06	9.14	M183	1 2 1 1 2	

(*continued*)

3421. $C_{15}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.905E-08	9.430E-06	10.80	M063	2 1 2 2 2	
4.900E-08	9.421E-06	10.80	M082	1 1 1 2 2	
4.900E-08	9.421E-06	10.80	M151	2 1 2 2 2	
4.909E-08	9.438E-06	10.84	M183	1 2 1 1 2	
5.773E-08	1.110E-05	13.90	M063	2 1 2 2 2	
5.750E-08	1.106E-05	13.90	M082	1 1 1 2 2	
5.750E-08	1.106E-05	13.90	M151	2 1 2 2 2	
5.778E-08	1.111E-05	13.94	M183	1 2 1 1 2	
7.542E-08	1.450E-05	18.30	M063	2 1 2 2 2	
7.540E-08	1.450E-05	18.30	M082	1 1 1 2 2	
7.540E-08	1.450E-05	18.30	M151	2 1 2 2 2	
7.550E-08	1.452E-05	18.34	M183	1 2 1 1 2	
9.934E-08	1.910E-05	23.10	M063	2 1 2 2 2	
9.940E-08	1.911E-05	23.10	M082	1 1 1 2 2	
9.940E-08	1.911E-05	23.10	M151	2 1 2 2 2	
9.944E-08	1.912E-05	23.14	M183	1 2 1 1 2	
2.028E-07	3.900E-05	25	M064	1 1 2 2 1	
1.108E-07	2.130E-05	25.00	M151	2 1 1 2 2	
1.259E-07	2.420E-05	27.00	M063	2 1 2 2 2	
1.260E-07	2.423E-05	27.00	M082	1 1 1 2 2	
1.260E-07	2.423E-05	27.00	M151	2 1 2 2 2	
1.260E-07	2.423E-05	27.04	M183	1 2 1 1 2	
1.670E-07	3.210E-05	31.10	M063	2 1 2 2 2	
1.670E-07	3.211E-05	31.10	M082	1 1 1 2 2	
1.670E-07	3.211E-05	31.10	M151	2 1 2 2 2	
1.671E-07	3.213E-05	31.14	M183	1 2 1 1 2	

3422. $C_{15}H_{12}$

9-Methylanthracene

RN: 779-02-2 **MP** (°C)**:** 79
MW: 192.26 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-06	2.610E-04	25	M064	1 1 2 2 2	
1.330E-06	2.557E-04	25	M342	1 0 1 1 2	
1.358E-06	2.610E-04	ns	M344	0 0 0 0 2	

3423. $C_{15}H_{12}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid benzyl ester
Benzyl 2,4-dichlorophenoxyacetate
2,4-DBE

RN: 13246-97-4 **MP** (°C)**:**
MW: 311.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.955E-05	1.542E-02	ns	M120	0 0 1 1 2	

3424. $C_{15}H_{12}Cl_2O_3$

Ethanol, 2-(2,4-dicholrophenoxy)-, benzoate
Benzoate, 2-(2,4-dichlorophenoxy)ethyl-
2,4-DEB
RN: 94-83-7 **MP** (°C)**:** 74
MW: 311.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-04	4.800E-02	ns	B185	0 0 0 0 0	

3425. $C_{15}H_{12}I_3NO_4$

Liothyronine
3,3′,5-Triiodothyronine
RN: 6893-02-3 **MP** (°C)**:** 236dec
MW: 650.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.080E-06	3.958E-03	37	L094	2 0 0 1 2	pH 4-5, zwitterion

3426. $C_{15}H_{12}N_2O$

5H-Dibenz[b,f]azepine-5-carboxamide
Carbazepine
5-Carbamoyl-5H-dibenz[b,f]azepine
Iminostilbene
Carbamazepine
Epitol
RN: 298-46-4 **MP** (°C)**:** 190–193
MW: 236.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.655E-04	1.100E-01	20	B196	0 0 0 0 0	
4.700E-04	1.110E-01	20	B196	0 0 0 0 0	
6.349E-04	1.500E-01	25	C437	0 0 0 0 0	Average
1.864E-03	4.404E-01	32	F425	0 0 0 0 0	pH 7.4
1.100E-03	2.600E-01	amb	L434	0 0 0 0 0	
4.232E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.000E-03	9.451E-01	rt	B397	0 0 0 0 0	EFG

3427. $C_{15}H_{12}N_2O_2$

Phenytoin
5,5-Diphenyl-2,4-imidazolidinedione
Dilantin
5,5-Diphenylhydantoin
Ekko
Zentropil

RN: 57-41-0 **MP** (°C)**:** 296.5
MW: 252.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.765E-04	9.499E-02	0	B114	1 1 1 2 1	pH 6-7
1.268E-04	3.200E-02	22	B154	1 1 1 1 1	0.1M HCl
7.531E-05	1.900E-02	25	A408	2 0 1 2 0	int
5.549E-05	1.400E-02	25	P061	0 0 0 0 0	pH 1-7
1.526E-04	3.850E-02	37	F183	1 0 1 1 2	intrinsic
2.600E-04	6.559E-02	50	M335	1 0 2 1 2	pH 5
2.323E-04	5.860E-02	ns	K446	0 0 0 0 0	
7.650E-05	1.930E-02	rt	I404	0 0 0 0 0	Average

3428. $C_{15}H_{12}N_2O_2$

Disperse violet 4
1-Amino-4-(*N*-methylamino)anthraquinone
Interchem acetate violet 6B

RN: 1220-94-6 **MP** (°C)**:** 193
MW: 252.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	5.802E-04	25	B333	0 0 0 0 0	

3429. $C_{15}H_{12}N_2O_3$

5-Phenyl-5-(*p*-hydroxy)phenyl-hydantoin
DL-5-(*p*-Hydroxyphenyl-5-phenylhydantoin
p-Hydroxyphenytoin
Hydroxydiphenylhydantoin
p-Hydroxydiphenylhydantoin

RN: 2784-27-2 **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.342E-04	3.600E-02	37	F183	1 0 1 1 2	intrinsic

3430. $C_{15}H_{12}N_2O_3$

Furfurin
1H-Imidazole, 2,4,5-tri-2-furanyl-4,5-dihydro-
2-Imidazoline, 2,4,5-tri-2-furyl-
RN: 550-23-2 **MP** (°C)**:**
MW: 268.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.000E-01	8	F300	1 0 0 0 0	
2.870E-02	7.700E+00	100	F300	1 0 0 0 1	

3431. $C_{15}H_{12}O_4$

Benzoyl-*r*-mandelic acid
p-Benzoylmandelic acid
RN: 100915-04-6 **MP** (°C)**:** 177
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-02	5.074E+00	0	A043	1 2 1 1 1	
1.980E-02	5.074E+00	0	L035	1 2 2 1 1	
2.327E-02	5.964E+00	10	A043	1 2 1 1 1	
2.327E-02	5.964E+00	10	L035	1 2 2 1 1	
2.520E-02	6.458E+00	15	A043	1 2 1 1 1	
2.520E-02	6.458E+00	15	L035	1 2 2 1 1	
2.828E-02	7.247E+00	20	A043	1 2 1 1 1	
2.828E-02	7.247E+00	20	L035	1 2 2 1 1	
3.059E-02	7.838E+00	25	A043	1 2 1 1 1	
3.059E-02	7.838E+00	25	L035	1 2 2 1 1	
3.557E-02	9.116E+00	30	A043	1 2 1 1 1	
3.557E-02	9.116E+00	30	L035	1 2 2 1 1	
4.017E-02	1.029E+01	35	A043	1 2 1 1 2	
4.017E-02	1.029E+01	35	L035	1 2 2 1 2	
4.894E-02	1.254E+01	40	A043	1 2 1 1 2	
4.894E-02	1.254E+01	40	L035	1 2 2 1 2	
6.032E-02	1.546E+01	45	A043	1 2 1 1 2	
6.032E-02	1.546E+01	45	L035	1 2 2 1 2	
7.201E-02	1.845E+01	50	A043	1 2 1 1 2	
7.201E-02	1.845E+01	50	L035	1 2 2 1 2	

3432. $C_{15}H_{12}O_4$

Benzoic acid, 2-(acetyloxy)-, phenyl ester
Phennin
Phenyl 2-acetoxybenzoate
Vesipyrin
Spiroform
Phenyl acetylsalicylate

RN: 134-55-4 **MP** (°C)**:** 97.5
MW: 256.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.805E-05	2.000E-02	21	N335	0 0 0 0 0	

3433. $C_{15}H_{13}Cl_3O_2$

2-*p*-Methoxyphenyl-2-*p*-hydroxyphenyl-1,1,1-trichloro-ethane
Phenol, 4-[2,2,2-trichloro-1-(4-methoxyphenyl)ethyl]-

RN: 28463-03-8 **MP** (°C)**:** 112–114
MW: 331.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-06	8.000E-04	ns	K117	0 1 2 1 1	

3434. $C_{15}H_{13}FO_2$

Flurbiprofen
3-Fluoro-4-phenylhydratropic acid
Froben
Ansaid

RN: 5104-49-4 **MP** (°C)**:** 110
MW: 244.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-05	6.180E-03	5	F306	1 0 1 2 2	intrinsic
2.761E-05	6.744E-03	24.99	K447	0 0 0 0 0	pH 2.0
4.339E-05	1.060E-02	25	A408	2 0 1 2 0	int
5.000E-05	1.221E-02	25	A411	1 0 0 1 0	int
1.332E-04	3.254E-02	25	C314	0 0 0 0 0	
1.331E-04	3.250E-02	25	C314	0 0 0 0 0	
3.870E-05	9.453E-03	25	F306	1 0 1 2 2	intrinsic
1.940E-04	4.739E-02	25	O303	1 0 0 1 0	EFG
4.600E-05	1.124E-02	37	F306	1 0 1 2 2	intrinsic
2.866E-05	7.000E-03	37	Y421	0 0 0 0 0	
>2.05E-03	>5.00E-01	ns	B404	0 2 1 1 0	
2.700E-04	6.595E-02	ns	O304	0 0 1 2 2	
3.275E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic

3435. $C_{15}H_{13}F_3N_4O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methyl-4-(trifluoromethyl)-

RN: 135794-72-8 **MP** (°C)**:**
MW: 322.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.209E-05	2.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3436. $C_{15}H_{13}NO$

7-Benzoylindoline
U-26,952

RN: 33244-57-4 **MP** (°C)**:** 124
MW: 223.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-05	2.290E-03	25	C046	0 0 0 0 0	

3437. $C_{15}H_{13}NO_2$

Dibenz[b,f][1,4]oxazepin-11(10H)-one, 10-ethyl-

RN: 17296-50-3 **MP** (°C)**:**
MW: 239.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.089E-04	4.999E-02	ns	M381	0 1 1 1 2	pH 7.0

3438. $C_{15}H_{13}NO_2S$

Metiazinic acid
Methiazinic acid

RN: 13993-65-2 **MP** (°C)**:** 146
MW: 271.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	3.100E-02	30	D015	2 0 1 1 0	EFG
2.211E-04	6.000E-02	37	D015	2 0 1 1 0	EFG

3439. $C_{15}H_{13}NO_3$

Ketorolac

RN: 74103-06-3 **MP** (°C)**:**
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.167E-04	1.830E-01	32	C411	2 1 1 2 1	
4.309E-04	1.100E-01	37	Y421	0 0 0 0 0	

3440. $C_{15}H_{13}NO_3$

Benzoyl acetaminophen
Acetamide, *N*-[4-(benzoyloxy)phenyl]-
Acetanilide, 4′-hydroxy-, benzoate (ester)
RN: 537-52-0 **MP** (°C)**:** 170.5–171.5
MW: 255.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-05	1.700E-02	37	D029	0 0 0 0 0	

3441. $C_{15}H_{13}NO_4$

Phenyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl phenyl ester
Acetanilide, 4′-hydroxy-, phenyl carbonate (ester)
RN: 17239-23-5 **MP** (°C)**:** 139–140.5
MW: 271.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-04	6.300E-02	37	D029	0 0 0 0 0	

3442. $C_{15}H_{13}N_3O_4S$

Piroxicam
2H-1,2-Benzothiazine-3-carboxamide, 4-hydroxy-2-methyl-*N*-2-pyridinyl-, 1,1-dioxide
Fensaid
Feldene
Candyl
Mobilis
RN: 36322-90-4 **MP** (°C)**:** 198
MW: 331.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-04	8.400E-02	25	M457	0 0 0 0 0	
1.608E-04	5.330E-02	32	C411	2 1 1 2 1	
<3.02E-04	<1.00E-01	rt	B435	0 0 0 0 0	
6.941E-05	2.300E-02	rt	H302	0 0 2 1 2	intrinsic

3443. $C_{15}H_{14}ClN_3O_4S$

Cefaclor
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2*R*)-aminophenylacetyl]amino]-3-chloro-8-oxo-, (6*R*,7*R*)-
Ceclor
Alfacet
Cephaclor
RN: 53994-73-3 **MP** (°C)**:**
MW: 367.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-02	1.000E+01	ns	L099	0 0 0 0 0	

3444. $C_{15}H_{14}ClN_3O_4S_3$

Benzthiazide
Exna
Hydrex
RN: 91-33-8 **MP** (°C)**:**
MW: 431.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.547E-05	1.100E-02	ns	B404	0 2 1 1 0	
6.482E-06	2.800E-03	rt	I404	0 0 0 0 0	Intrinsic, Average

3445. $C_{15}H_{14}Cl_2F_3N_3O_3$

Carfentrazone-ethyl
Df herbicide
Benzenepropanoic acid, α-2-dichloro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}-4-fluoro-, ethyl ester
Ethyl 2-chloro-3-{2-chloro-4-fluoro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}phenyl}propanoate
F 8426
RN: 128639-02-1 **MP** (°C)**:**
MW: 412.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.333E-05	2.198E-02	ns	S460	0 0 0 0 0	

3446. $C_{15}H_{14}Cl_2N_4O_3$
C.I. Disperse orange 5
Ethanol, 2-[[4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]methylamino]
Amacel fast brown 3R
Celliton fast brown 3R
RN: 6232-56-0 **MP** (°C)**:** 127
MW: 369.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-07	1.588E-04	25	B333	0 0 0 0 0	
8.938E-06	3.300E-03	60	P313	0 0 0 0 0	average of 2
1.530E-05	5.650E-03	70	P313	0 0 0 0 0	average of 2
2.939E-05	1.085E-02	80	P313	0 0 0 0 0	average of 2
6.378E-05	2.355E-02	90	P313	0 0 0 0 0	average of 2
1.354E-04	5.000E-02	100	P313	0 0 0 0 0	

3447. $C_{15}H_{14}F_3N_3O_4S_2$
Bendroflumethiazide
Corzide
Rauzide
Naturetin
RN: 73-48-3 **MP** (°C)**:** 222
MW: 421.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	5.057E-02	20	A080	1 0 2 1 2	
2.570E-04	1.083E-01	25	A076	1 0 1 1 2	
2.847E-05	1.200E-02	ns	B404	0 2 1 1 0	
9.492E-05	4.000E-02	rt	A095	0 0 2 2 0	
3.631E-05	1.530E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

3448. $C_{15}H_{14}NO_2PS$
Cyanofenphos
O-(4-Cyanophenyl) *O*-ethyl phenylphosphonothioate
Surecide
RN: 13067-93-1 **MP** (°C)**:** 83
MW: 303.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-06	6.000E-04	30	M161	1 0 0 0 0	

3449. $C_{15}H_{14}N_2O_2$
Dibenz[b,f][1,4]oxazepin-11(10H)-one, 8-amino-2-methyl-
RN: 155206-47-6 **MP** (°C)**:**
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-04	3.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3450. $C_{15}H_{14}N_2O_3$
p-(3-Phenylureido)phenyl acetate
Benzeneacetic acid, 4-[[(phenylamino)carbonyl]amino]-
RN: 181518-40-1 **MP** (°C)**:**
MW: 270.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	9.730E-03	25	A066	1 0 1 1 1	

3451. $C_{15}H_{14}N_2O_5$
2′-Ethoxy-2hydroxy-5-nitrobenzanilide
Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-5-nitro-
RN: 213460-67-4 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-05	5.098E-03	25	D400	2 0 0 1 2	

3452. $C_{15}H_{14}N_2O_5$
4′-Ethoxy-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(4-ethoxyphenyl)-2-hydroxy-3-nitro-
RN: 213460-61-8 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:** 342.2–426.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.119E-05	9.428E-03	25	D400	2 0 0 1 2	

3453. $C_{15}H_{14}N_2O_5$
2′-Ethoxy-2-hydroxy-3-nitrobenzanilide
Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-3-nitro-
RN: 213460-63-0 **MP** (°C)**:**
MW: 302.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-05	7.352E-03	25	D400	2 0 0 1 2	

3454. $C_{15}H_{14}N_4O$
Nevarapine
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-4-methyl
Nevirapine
BI-RG 587
RN: 129618-40-2 **MP** (°C)**:** 248
MW: 266.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-04	1.000E-01	ns	K444	0 0 0 0 0	
6.412E-04	1.708E-01	ns	M381	0 1 1 1 2	pH 7.0

3455. $C_{15}H_{14}O_3$
Methyl benzoyl benzoate
Benzoic acid, 4-hydroxy-, (4-methylphenyl)methyl ester
RN: 84833-58-9 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.064E-04	5.000E-02	ns	F014	0 0 0 0 0	

3456. $C_{15}H_{14}O_3$
[4-(Benzyloxy)phenyl]acetic acid
(4-Boph)
RN: 6547-53-1 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.711E-04	6.568E-02	20	K437	0 0 0 0 0	pH 2.0
3.711E-04	8.990E-02	25	K437	0 0 0 0 0	pH 2.0
6.338E-04	1.536E-01	30	K437	0 0 0 0 0	pH 2.0
7.293E-04	1.767E-01	37	K437	0 0 0 0 0	pH 2.0

3457. $C_{15}H_{14}O_3$
Fenoprofen
Fenoporfen
Progesic
Fenpron
Nalfon
Fenopron
RN: 31879-05-7 **MP** (°C)**:**
MW: 242.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-04	1.000E-01	37	Y421	0 0 0 0 0	

3458. $C_{15}H_{15}ClF_3N_3O$

Triflumizole

RN: 99387-89-0 **MP** (°C)**:** 63.5
MW: 345.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.480E-05	1.549E-02	25	V410	0 0 0 0 0	

3459. $C_{15}H_{15}ClN_2O_2$

Chlorooxuron
(*N′*-4-(4-Chlorophenoxy)phenyl-*N,N*-dimethylurea)
3-[*p*-(*p′*-Chlorophenoxy)phenyl]-1,1-dimethylurea
N-4-(4′-Chlorophenoxy)phenyl-*N′,N′*-dimethylurea
Tenoran

RN: 1982-47-4 **MP** (°C)**:** 151
MW: 290.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-05	3.700E-03	20	B185	0 0 0 0 0	
1.273E-05	3.700E-03	20	G036	1 0 0 0 1	
1.273E-05	3.700E-03	20	M161	1 0 0 0 1	pH 7
9.286E-06	2.700E-03	ns	B200	0 0 0 0 1	
1.273E-04	3.700E-02	ns	M061	0 0 0 0 1	

3460. $C_{15}H_{15}ClN_2O_4S$

Xipamide
2′,6′-Salicyloxylidide, 4-chloro-5-sulfamoyl-
Aquaphor
Aquaphor (diuretic)
BEI 1293
Diurex

RN: 14293-44-8 **MP** (°C)**:** 256
MW: 354.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.635E-04	5.800E-02	25	H074	1 2 2 1 1	

3461. $C_{15}H_{15}ClN_4O_6S$

Chlorimuron-ethyl
Chlorimuron ethyl ester
Classic 75DF
Classic
Chlorimuron Et
2-[[[[(4-Chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]benzoic acid ethyl ester
RN: 90982-32-4 **MP** (°C)**:** 180–182
MW: 414.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.455E-06	1.018E-03	ns	R427	0 0 0 0 0	

3462. $C_{15}H_{15}ClO$

2-Benzyl-3,5-dimethyl-4-chloro-phenol
RN: 1867-85-2 **MP** (°C)**:**
MW: 246.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.234E-02	25	B316	0 0 0 0 0	

3463. $C_{15}H_{15}NO_2$

Mefenamic acid
2′,3′-Dimethyl-*N*-phenyl-anthranilic acid
Forte mefenamic acid
N-(2,3-Xylyl)anthranilic acid
Ponstel
Ponstan
RN: 61-68-7 **MP** (°C)**:** 230.5
MW: 241.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.289E-05	2.000E-02	30	D015	2 0 1 1 0	EFG
2.800E-05	6.756E-03	35	H091	1 2 2 2 1	*sic*
1.658E-04	4.000E-02	37	D015	2 0 1 1 0	EFG
1.658E-06	4.000E-04	37	P432	0 0 0 0 0	
1.227E-04	2.960E-02	37	P432	0 0 0 0 0	
8.289E-07	2.000E-04	37	Y421	0 0 0 0 0	
1.100E-04	2.654E-02	ns	O304	0 0 1 2 2	

3464. $C_{15}H_{15}NO_3$
Tolmetin
Tolectin
RN: 26171-23-3 **MP** (°C)**:**
MW: 257.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-05	2.000E-02	37	Y421	0 0 0 0 0	

3465. $C_{15}H_{15}N_3O$
5H-Pyrido[2,3-b][1,5]benzodiazepine-5-one, 11-ethyl-6,11-dihydro-6-methyl-
RN: 132686-75-0 **MP** (°C)**:**
MW: 253.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.782E-05	4.515E-03	ns	M381	0 1 1 1 2	pH 7.0
4.742E-04	1.201E-01	ns	M381	0 1 1 1 2	pH 7.0

3466. $C_{15}H_{15}N_3O_2$
Pyrido[2,3-b][1,5]benzoxazepin-5(6H)-one, 3-amino-6,7,9-trimethyl-
RN: **MP** (°C)**:**
MW: 269.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	4.658E-02	ns	M381	0 1 1 1 2	pH 7.0

3467. $C_{15}H_{15}N_3O_2$
C.I. Disperse yellow 3
Acetamide, *N*-[4-[(2-hydroxy-5-methylphenyl)azo]phenyl]-
RN: 2832-40-8 **MP** (°C)**:** 195
MW: 269.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.232E-05	25	B333	0 0 0 0 0	

3468. $C_{15}H_{15}N_3S$
5H-Pyrido[2,3-b][1,5]benzodiazepine-5-thione, 11-ethyl-6,11-dihydro-6-methyl-
RN: 132686-95-4 **MP** (°C)**:**
MW: 269.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.968E-05	5.301E-03	ns	M381	0 1 1 1 2	pH 7.0

3469. $C_{15}H_{16}N_2O_2$
Ancymidol
α-Cyclopropyl-α-(4-methoxyphenyl)-5-pyrimidinemethanol
A-Rest
RN: 12771-68-5 **MP** (°C)**:** 110.5
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-03	6.500E-01	25	M161	1 0 0 0 2	

3470. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 5,11-dihydro-5-methyl-11-propyl-
RN: 132312-81-3 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-03	3.562E-01	ns	M381	0 1 1 1 2	pH 7.0

3471. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2,4-dimethyl-
RN: 134698-31-0 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.793E-05	7.493E-03	ns	M381	0 1 1 1 2	pH 7.0

3472. $C_{15}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 5,11-diethyl-5,11-dihydro-
RN: 132312-82-4 **MP** (°C)**:**
MW: 268.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-03	3.704E-01	ns	M381	0 1 1 1 2	pH 7.0

3473. $C_{15}H_{16}N_4O_2$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methoxy-4-methyl-
RN: 135794-75-1 **MP** (°C)**:**
MW: 284.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-06	1.999E-03	ns	M381	0 1 1 1 2	pH 7.0

3474. $C_{15}H_{16}N_4O_2$

1H-Purine-2,6-dione, 1,3-diethyl-3,7-dihydro-8-phenyl-
1,3-Diethyl-8-phenylxanthine
8-Phenyl-1,3-diethylxanthine

RN: 75922-48-4 **MP** (°C)**:**
MW: 284.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.517E-06	1.000E-03	ns	H316	0 0 0 0 0	0.1N HCL
2.110E-05	6.000E-03	ns	H316	0 0 0 0 0	pH 7.4

3475. $C_{15}H_{16}N_4O_5S$

Benzenesulfonic acid, 4-(1,3-Diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-

RN: 89073-47-2 **MP** (°C)**:** >360
MW: 364.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.56E-01	>5.70E+01	ns	H316	0 0 0 0 0	pH 7.4
>2.20E-02	>8.00E+00	ns	H316	0 0 0 0 0	0.1N HCL

3476. $C_{15}H_{16}O_2$

Bisphenol A
2,2-*bis*-[4-Hydroxyphenyl]-propan
2,2-*bis*-(4-Hydroxypheny)-propane

RN: 80-05-7 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.533E-03	3.500E-01	20	F300	1 0 0 0 1	
4.775E-04	1.090E-01	22	Y419	0 0 0 0 0	
1.314E-03	3.000E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	25	D415	1 0 0 0 0	
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	
1.314E-03	3.000E-01	25	S468	0 0 0 0 0	

3477. $C_{15}H_{16}O_2$
Bisphenol A
RN: 80-05-7 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	

3478. $C_{15}H_{16}O_2$
Nabumetone
RN: 42924-53-8 **MP** (°C)**:**
MW: 228.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.628E-05	6.000E-03	22.5	C438	0 0 0 0 0	

3479. $C_{15}H_{16}O_3$
Osthole
2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methyl-2-butenyl)-
RN: 484-12-8 **MP** (°C)**:** 83.5
MW: 244.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.912E-05	1.200E-02	30	B144	1 0 1 0 1	

3480. $C_{15}H_{16}O_9.2H_2O$
Aesculin (dihydrate)
Esculin
6,7-Dihydroxycoumarin 6-glucoside
2H-1-Benzopyran-2-one, 6-(β-D-glucopyranosyloxy)-7-hydroxy-
RN: 531-75-9 **MP** (°C)**:** 205dec
MW: 376.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.605E-03	1.733E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3481. $C_{15}H_{17}FN_4O_2$

Flupirtine

Carbamic acid, [2-amino-6-[[(4-fluorophenyl)methyl]amino]-3-pyridinyl]-, ethyl ester

RN: 56995-20-1 **MP** (°C)**:** 175.8–177.7

MW: 304.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.286E-03	1.000E+00	ns	D321	0 0 0 0 0	

3482. $C_{15}H_{17}NO_3$

Acetamide, 2-(benzoyloxy)-*N,N*-di-acetamide, 2-(benzoyloxy)-*N,N*-di-2-propenyl-

RN: 106231-58-7 **MP** (°C)**:** 42.5

MW: 259.31 **BP** (°C)**:** 401.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.738E-03	7.100E-01	22	B427	1 0 0 1 1	in 0.01M HCl
2.738E-03	7.100E-01	22	N317	1 1 2 1 2	

3483. $C_{15}H_{17}NO_5$

L-Proline, 1-[(benzoyloxy)acetyl]-, methyl ester

RN: 115178-76-2 **MP** (°C)**:** 72.5

MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.239E-03	2.400E+00	22	N317	1 1 2 1 2	

3484. $C_{15}H_{17}NO_7$

Glycine, *N*-[[[2-(acetyloxy)benzoyl]oxy]acetyl]-, ethyl ester

RN: 118247-03-3 **MP** (°C)**:** 68.5

MW: 323.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.320E+00	21	N335	0 0 0 0 0	

3485. $C_{15}H_{17}N_3O_3S$
L-Ala-dapsone
2-Amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-propanamide
RN: 160348-99-2 **MP** (°C)**:**
MW: 319.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.066E-02	6.600E+00	25	P351	0 0 0 0 0	pH 7.4
>9.39E-02	>3.00E+01	25	P351	0 0 0 0 0	

3486. $C_{15}H_{18}Cl_2N_2O_3$
Oxadiazon
3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one
Ronstar
Scotts OH I
RP-17623
RN: 19666-30-9 **MP** (°C)**:** 88
MW: 345.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-06	7.000E-04	20	M161	1 0 0 0 0	
2.028E-06	7.000E-04	24	C105	2 1 2 2 2	

3487. $C_{15}H_{18}I_3NO_5$
Iopronic acid
Butanoic acid, 2-[[2-[3-(acetylamino)-2,4,6-triiodophenoxy]ethoxy]methyl]-
RN: 37723-78-7 **MP** (°C)**:** 130
MW: 673.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.984E-02	2.008E+01	37	J016	1 0 0 0 2	pH 7.4
1.456E-04	9.799E-02	50	F013	1 0 1 1 1	

3488. $C_{15}H_{18}N_2O_3$
N-Acetyl-L-tryptophan ethyl ester
RN: 2382-80-1 **MP** (°C)**:** 106
MW: 274.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-03	5.200E-01	5	L081	2 2 2 2 1	
5.359E-03	1.470E+00	28	L081	2 1 2 2 2	

3489. $C_{15}H_{18}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-ethyl-5-methylpyrimidine

RN: **MP** (°C)**:**

MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.077E-05	3.600E-03	37	R076	1 2 0 0 1	

3490. $C_{15}H_{18}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-*n*-propylpyrimidine

RN: **MP** (°C)**:**

MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.914E-05	6.400E-03	37	R076	1 2 0 0 2	

3491. $C_{15}H_{18}N_4O_5$

Mitomycin C

MMC

6-Amino-8-[[(aminocarbonyl)oxy]methyl]-1,1α,2,8,8α,8β-hexahydro-8α-methoxy-5-methyl,[1a*S*-(1α,8β,8aα,8bα)]-azirino[2′,3′:3,4]pyrrolo[1,2a]indole-4,7-dione

Mitomycinum

RN: 50-07-7 **MP** (°C)**:** >360

MW: 334.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.730E-03	9.127E-01	25	M316	1 1 1 1 2	
8.500E-01	2.842E+02	ns	B406	0 0 2 2 0	EFG

3492. $C_{15}H_{18}O_3$

Santonin

Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3α,5,5α,9β-tetrahydro-3,5α,9-trimethyl-, (3*S*,3α*S*,5α*S*,9β*S*)-

RN: 481-06-1 **MP** (°C)**:** 170

MW: 246.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-04	2.000E-01	17.5	F300	1 0 0 0 0	
1.624E-02	4.000E+00	100	F300	1 0 0 0 0	

3493. $C_{15}H_{18}O_4$

β-Cyclopentylpropionyl salicylate

RN: **MP** (°C)**:**

MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	2.780E-02	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.91, intrinsic

3494. $C_{15}H_{19}ClO_2$

1,1-Drichloro-1-methyl-2,2-bis(*p*-methoxylphenyl)ethane

RN: 56288-27-8 **MP** (°C)**:**

MW: 266.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-06	1.700E-03	rt	C122	0 0 0 0 0	

3495. $C_{15}H_{19}NO$

N,N-Hexamethylenecinnamamide

Hexahydro-1-(1-oxo-3-phenyl-2-propenyl)1H-azepine

RN: 59832-05-2 **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	5.641E-02	ns	H350	0 0 0 0 0	

3496. $C_{15}H_{19}NO$

N-Cyclohexylcinnamamide

2-Propenamide, *N*-cyclohexyl-3-phenyl-

RN: 6750-98-7 **MP** (°C)**:**

MW: 229.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-05	9.265E-03	ns	H350	0 0 0 0 0	

3497. $C_{15}H_{19}NO_2$
Tropacocaine
RN: 537-26-8 **MP** (°C)**:** 49
MW: 245.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.055E+00	15	K059	2 2 2 0 1	

3498. $C_{15}H_{19}NO_3$
1H-Azepine, 1-[(benzoyloxy)acetyl]hexahydro-
RN: 115178-68-2 **MP** (°C)**:** 107.5
MW: 261.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E-03	7.500E-01	22	N317	1 1 2 1 2	

3499. $C_{15}H_{19}NO_5$
Benzoic acid, 2-(acetyloxy)-, 2-(diethylamino)-2-oxoethyl ester
RN: 116482-56-5 **MP** (°C)**:** 76.5
MW: 293.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-03	2.280E+00	21	N335	0 0 0 0 0	

3500. $C_{15}H_{20}N_2O_4$
Benzyl-2,2-diethylmalonurate
Benzyl 2,2-diethylmalonurate

RN: 73632-78-7 **MP** (°C): 107
MW: 292.34 **BP** (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	6.431E-02	23	B152	1 2 1 1 1	pH 3.5

3501. $C_{15}H_{20}N_2O_4S$
Acetohexamide
Acetohexamid
1-(*p*-Acetylbenzenesulfonyl)-3-cyclohexylurea
Dymelor
Dimelin
RN: 968-81-0 **MP** (°C)**:** 189
MW: 324.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.706E-04	2.500E-01	25	K023	1 0 2 2 1	EFG, pH 6.5, average of 2
3.483E-05	1.130E-02	37	B130	1 2 1 1 2	pH 1.5, form II
4.963E-05	1.610E-02	37	B130	1 2 1 1 2	pH 1.5, form III
8.015E-05	2.600E-02	37	K106	1 2 2 2 0	EFG, form I
9.556E-05	3.100E-02	37	K106	1 2 2 2 0	EFG, form II

3502. $C_{15}H_{20}N_4O_2S$
2-Sulfanilylamino-4-amylpyrimidine
RN: 107203-72-5 **MP** (°C)**:**
MW: 320.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-04	2.000E-01	37	R076	1 2 0 0 1	

3503. $C_{15}H_{20}N_4O_5$
1,5-Dibutyryloxymethyl allopurinol
RN: 98827-19-1 **MP** (°C)**:** 122–123
MW: 336.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-04	5.000E-02	22	B322	0 0 0 0 0	

3504. $C_{15}H_{20}N_4O_5$
2,5-Dibutyryloxymethyl allopurinol
RN: 98827-20-4 **MP** (°C)**:** 133–135
MW: 336.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.795E-04	9.400E-02	22	B322	0 0 0 0 0	

3505. $C_{15}H_{20}N_4O_6$
9-[5-*O*-(Butyrate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine
RN: 121032-41-5 **MP** (°C)**:** 108–110
MW: 352.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.680E-03	3.411E+00	37	M378	1 2 1 1 2	pH 7.2

3506. $C_{15}H_{20}N_4O_6.0.3H_2O$
2′-Butyryl-6-methoxypurine arabinoside (0.3 hydrate)
RN: 121032-41-5 **MP** (°C)**:**
MW: 357.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-01	8.264E+01	37	C348	0 0 0 0 0	pH 7.00

3507. $C_{15}H_{20}N_4O_6$
2′-Isobutyryl-6-methoxypurine arabinoside
RN: 121032-44-8 **MP** (°C)**:**
MW: 352.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	2.361E+02	37	C348	0 0 0 0 0	pH 7.00

3508. $C_{15}H_{20}N_4O_6.0.25H_2O$
9-[5-*O*-(Isobutyrate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)
RN: 121032-44-8 **MP** (°C)**:** glass
MW: 356.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	1.367E+01	37	M378	1 2 1 1 2	pH 7.2

3509. $C_{15}H_{21}NO$
N,N-Dipropylcinnamamide
Cinnamamide, *N,N*-dipropyl-
RN: 23784-56-7 **MP** (°C)**:**
MW: 231.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.890E-03	6.686E-01	ns	H350	0 0 0 0 0	

3510. $C_{15}H_{21}NO_2$
Meperidine
Ethyl 1-methyl-4-phenylpiperidine-4-carboxylate
Demerol
Dolantin
Pethidine
RN: 57-42-1 **MP** (°C)**:** 30
MW: 247.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.648E-02	6.550E+00	25	R338	0 0 0 0 0	
1.300E-02	3.215E+00	30	L068	1 0 0 1 0	EFG

3511. $C_{15}H_{21}NO_2S_2$
2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dithiolane
RN: 35801-67-3 **MP** (°C)**:**
MW: 311.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	7.787E-03	rt	B174	0 0 1 0 1	

3512. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-bis(1-methylethyl)-
RN: 106231-56-5 **MP** (°C)**:** 105.5
MW: 263.34 **BP** (°C)**:** 391.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.557E-04	1.200E-01	22	B427	1 0 0 1 1	in 0.01M HCl
4.557E-04	1.200E-01	22	N317	1 1 2 1 2	

3513. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N*-hexyl-
RN: 115193-29-8 **MP** (°C)**:** 130.5
MW: 263.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	3.300E-02	22	N317	1 1 2 1 2	

3514. $C_{15}H_{21}NO_3$
Acetamide, 2-(benzoyloxy)-*N,N*-dipropyl-
RN: 106231-55-4 **MP** (°C)**:** 20
MW: 263.34 **BP** (°C)**:** 402.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.177E-03	1.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.177E-03	1.100E+00	22	N317	1 1 2 1 2	

3515. $C_{15}H_{21}NO_3S$

2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-oxathiolane

RN: 24606-94-8 **MP** (°C)**:**
MW: 295.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.772E-02	rt	B174	0 0 1 0 0	

3516. $C_{15}H_{21}NO_4$

Metalaxyl
Methyl *N*-(2,6-dimethyl-phenyl)-*N*-(2′-methoxyacetyl)-DL-alaninate
Apron
Ridomil
Subdue
Fubol

RN: 57837-19-1 **MP** (°C)**:** 72
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.951E+00	20	E048	1 2 1 1 2	

3517. $C_{15}H_{21}NO_4$

Hexyl acetaminophen
Carbonic acid, 4-(acetylamino)phenyl hexyl ester
Acetanilide, 4′-hydroxy-, hexyl carbonate (ester)

RN: 17239-22-4 **MP** (°C)**:** 112.5-113.5
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-04	3.700E-02	37	D029	0 0 0 0 0	

3518. $C_{15}H_{21}NO_4$

2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dioxolane

RN: 35858-24-3 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.514E-01	rt	B174	0 0 1 0 0	

3519. $C_{15}H_{21}NO_5$

Acetamide, 2-(benzoyloxy)-*N,N*-bis(2-methoxyethyl)-

RN: 115178-64-8 **MP** (°C)**:** 57.5
MW: 295.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-02	7.890E+00	22	N317	1 1 2 1 2	

3520. $C_{15}H_{21}NO_5$
Acetamide, 2-(benzoyloxy)-*N*,*N*-bis(2-hydroxypropyl)-
RN: 115178-63-7 **MP** (°C)**:** 105.5
MW: 295.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.636E-02	1.960E+01	22	N317	1 1 2 1 2	

3521. $C_{15}H_{21}N_2O_3$
C.I. Disperse red 11
RN: 2872-48-2 **MP** (°C)**:** 242
MW: 277.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	6.934E-04	25	B333	0 0 0 0 0	

3522. $C_{15}H_{21}N_3O$
Primaquine
Primaquine phosphate
Neo-quipenyl
8-(4-Amino-1-methylbutylamino)-6-methoxyquinoline
8-((4-Amino-1-methylbutyl)amino)-6-methoxyquinoline phosphate
Palum
RN: 90-34-6 **MP** (°C)**:**
MW: 259.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.770E+00	7.184E+02	25	B443	0 0 0 0 0	

3523. $C_{15}H_{21}N_5O_5$
9-(2-*O*-Valeryl-β-D-arabinofuranosyl)adenine
RN: 87984-85-8 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.960E-04	1.040E-01	37	B306	1 2 0 1 2	pH 7.3

3524. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Isovaleryl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-32-1 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	1.980E+01	ns	B134	0 1 1 1 2	

3525. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Valeryl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-31-0 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.391E-02	8.400E+00	ns	B134	0 1 1 1 1	

3526. $C_{15}H_{21}N_5O_5$
9-[5′-(*O*-Pivaloyl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-33-2 **MP** (°C)**:**
MW: 351.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-02	7.000E+00	ns	B134	0 1 1 1 1	

3527. $C_{15}H_{21}N_5O_6$
9-(1,3-Dipropionate-2-propoxymethyl)guanine
RN: 86357-20-2 **MP** (°C)**:** 192
MW: 367.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.622E-03	2.800E+00	25	B360	0 0 0 0 0	

3528. $C_{15}H_{22}ClNO_2$
Metolachlor
2-Chloro-*N*-(2-ethyl-6-methylphenyl)-*N*-(2-methoxy-1-methylethyl)acetamide
Dual
Cotoran Multi
Ontrack 8E
Bicep 6L
RN: 51218-45-2 **MP** (°C)**:** <25
MW: 283.80 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.867E-03	5.297E-01	20	E048	1 2 1 1 2	
1.868E-03	5.300E-01	20	M161	1 0 0 0 2	
1.866E-03	5.297E-01	ns	S460	0 0 0 0 0	
1.868E-03	5.300E-01	ns	V414	0 0 0 0 0	

3529. $C_{15}H_{22}ClNO_2$

CP 52223
2-Chloro-*N*-(2,6-dimethyl)phenyl-*N*-isopropoxymethylacetamide
RN: 24353-58-0 **MP** (°C)**:**
MW: 283.80 **BP** (°C)**:** 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E-04	5.900E-02	ns	M061	0 0 0 0 1	

3530. $C_{15}H_{22}N_2O$

DL-Mepivacaine
Carbocaine
1-Methyl-2′,6′-pipecoloxylidide
Carbocain
RN: 96-88-8 **MP** (°C)**:** 150
MW: 246.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	3.350E+00	14.9	N046	2 0 1 1 1	intrinsic
3.653E-02	9.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
2.841E-02	7.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
9.000E-03	2.217E+00	25	D402	1 2 2 2 0	EFG
1.020E-02	2.513E+00	25	N046	2 0 1 1 1	intrinsic
9.910E-03	2.441E+00	34.5	N046	2 0 1 1 1	intrinsic
1.000E-02	2.464E+00	37	D402	1 2 2 2 0	EFG
7.970E-03	1.963E+00	37	N044	2 1 1 2 2	intrinsic

3531. $C_{15}H_{22}O_3$

Gemfibrozil
2,2-Dimethyl-5-(2,5-xylyloxy)valeric acid
Jezil
Lobid
Lopid
RN: 25812-30-0 **MP** (°C)**:**
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.00E-03	>5.00E-01	ns	B404	0 2 1 1 0	

3532. $C_{15}H_{22}O_3$

Octyl *p*-hydroxybenzoate
n-Octyl 4-hydroxybenzoate
RN: 1219-38-1 **MP** (°C)**:** 54
MW: 250.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-05	3.680E-03	15	B355	0 0 0 0 0	
2.300E-04	5.758E-02	20	B355	0 0 0 0 0	
4.650E-04	1.164E-01	25	B355	0 0 0 0 0	
3.273E-03	8.193E-01	25	D081	1 2 2 1 2	
3.162E-04	7.916E-02	25	F322	2 0 1 1 0	EFG

3533. $C_{15}H_{22}O_5$

Octyl gallate
Octyl 3,4,5-trihydroxybenzoate
n-Octyl gallate
RN: 1034-01-1 **MP** (°C)**:**
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.084E-05	2.000E-02	29.99	L430	0 0 0 0 0	
8.500E-05	2.400E-02	34.99	L430	0 0 0 0 0	
1.133E-04	3.200E-02	39.99	L430	0 0 0 0 0	
1.806E-04	5.100E-02	44.99	L430	0 0 0 0 0	
3.152E-04	8.899E-02	49.99	L430	0 0 0 0 0	
4.214E-04	1.190E-01	54.99	L430	0 0 0 0 0	
4.710E-04	1.330E-01	59.99	L430	0 0 0 0 0	
5.064E-04	1.430E-01	64.99	L430	0 0 0 0 0	

3534. $C_{15}H_{23}NO_2$

Octyl *m*-aminobenzoate
Octyl 3-aminobenzoate
RN: 52222-35-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	7.481E-03	ns	M066	0 0 0 0 0	

3535. $C_{15}H_{23}NO_2$

Octyl *p*-aminobenzoate
4-Aminobenzoic acid octyl ester
RN: 14309-41-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-06	7.979E-04	37	F006	1 1 2 2 1	

3536. $C_{15}H_{23}NO_2$

Alprenolol
Aptin
RN: 13655-52-2 **MP** (°C)**:**
MW: 249.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.471E-03	3.669E-01	22.5	B422	0 0 0 0 0	

3537. $C_{15}H_{23}NO_3$

Parethoxycaine
4-Ethoxybenzoic acid-2-(diethylamino)ethyl ester
RN: 94-23-5 **MP** (°C)**:** 173.0
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-03	5.121E-01	ns	M066	0 0 0 0 2	

3538. $C_{15}H_{23}NO_4$

Cycloheximide
3-((*R*)-2-((1*S*,3*S*,5*S*)-3,5-Dimethyl-2-oxocyclohexyl)-2-hydroxyethyl)glutarimide
Actidione
Actispray
Naramycin
Kaken
RN: 66-81-9 **MP** (°C)**:** 116.3
MW: 281.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.464E-02	2.100E+01	2	M161	1 0 0 0 1	

3539. $C_{15}H_{23}N_3O_4$

Isopropalin
2,6-Dinitro-*N,N*-dipropylcumidene
4-Isopropyl-2,6-dinitro-*N,N*-dipropylaniline
2,6-Dinitro-*N,N*-dipropylcumidine
Paarlan
Paarlan EC
RN: 33820-53-0 **MP** (°C)**:**
MW: 309.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.232E-07	1.000E-04	25	M161	1 0 0 0 0	

3540. $C_{15}H_{23}N_3O_4S$

Sulpiride

N-[(1-Ethyl-2-pyrrolidinyl)methyl]-2-methoxy-5-sulfamoylbenzamide

RN: 15676-16-1 **MP** (°C)**:**

MW: 341.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-04	<2.10E-01	25	P312	0 0 0 0 0	

3541. $C_{15}H_{23}N_3O_4S$

Cyclacillin

Anhydrous 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 **MP** (°C)**:**

MW: 341.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-01	5.500E+01	7	P035	0 0 0 0 0	EFG
1.054E-01	3.600E+01	20	P035	0 0 0 0 0	EFG
9.372E-02	3.200E+01	25	P035	0 0 0 0 0	EFG
7.908E-02	2.700E+01	30	P035	0 0 0 0 0	EFG
6.736E-02	2.300E+01	40	P035	0 0 0 0 0	EFG
6.151E-02	2.100E+01	50	P035	0 0 0 0 0	EFG
5.858E-02	2.000E+01	60	P035	0 0 0 0 0	EFG

3542. $C_{15}H_{23}N_3O_4S.2H_2O$

Cyclacillin (dihydrate)

Dihydrate 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 **MP** (°C)**:**

MW: 377.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	1.400E+01	10	P035	0 0 0 0 0	EFG
3.709E-02	1.400E+01	20	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	25	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	30	P035	0 0 0 0 0	EFG
3.682E-02	1.390E+01	40	P035	0 0 0 0 0	EFG
3.762E-02	1.420E+01	50	P035	0 0 0 0 0	EFG
4.504E-02	1.700E+01	60	P035	0 0 0 0 0	EFG

3543. $C_{15}H_{24}NO_4PS$

Isofenphos
Methylethyl 2-((ethoxy((1-methylethyl)amino)phosphinothioyl)oxy)benzoate
Amaze
Oftanol
Pryfon
RN: 25311-71-1 **MP** (°C)**:**
MW: 345.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-05	2.210E-02	20	B300	2 1 1 1 2	*sic*
6.891E-02	2.380E+01	20	M161	1 0 0 0 2	*sic*

3544. $C_{15}H_{24}N_2O_2$

N,N,N′-Triethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide
RN: 62249-37-0 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-01	5.900E+01	20	K050	1 1 1 1 2	

3545. $C_{15}H_{24}N_2O_2$

Tetracaine
Pantocaine
Cetacaine
RN: 94-24-6 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	1.560E-01	ns	E031	0 0 2 1 2	

3546. $C_{15}H_{24}N_2O_2$

4-Ethylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-53-2 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-03	1.216E+00	ns	M066	0 0 0 0 1	

3547. $C_{15}H_{24}N_2O_2$

4-Aminobenzoic acid-2-(diethyl-amino)butyl ester
2-(Diethyl(amino)butyl 4-aminobenzoate
RN: 5878-14-8 **MP** (°C)**:**
MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.137E+00	ns	M066	0 0 0 0 1	

3548. $C_{15}H_{24}N_2O_3$

2,4-Diazaspiro[5.11]heptadecane-1,3,5-trione
RN: 143288-64-6 **MP** (°C)**:**
MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-06	4.486E-04	25	P350	0 0 0 0 0	intrinsic

3549. $C_{15}H_{24}O$

Butylated hydroxytoluene
2,6-Di-*tert*-butyl-*p*-cresol
2,6-Di-*tert*-butyl-1-hydroxy-4-methylbenzene
4-Hydroxy-3,5-di-*tert*-butyltoluene
RN: 128-37-0 **MP** (°C)**:** 71
MW: 220.36 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.54E-05	<1.00E-02	25	P312	0 0 0 0 0	

3550. $C_{15}H_{24}O$

4-Nonylphenol
4-*t*-Nonylphenol
RN: 104-40-5 **MP** (°C)**:**
MW: 220.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-05	4.605E-03	2	A335	0 0 0 0 0	
2.088E-05	4.600E-03	2	A335	0 0 0 0 0	
2.230E-05	4.914E-03	10	A335	0 0 0 0 0	
2.233E-05	4.920E-03	10	A335	0 0 0 0 0	
2.380E-05	5.245E-03	14	A335	0 0 0 0 0	
2.378E-05	5.240E-03	14	A335	0 0 0 0 0	
2.470E-05	5.443E-03	20.5	A335	0 0 0 0 0	
2.464E-05	5.430E-03	20.5	A335	0 0 0 0 0	
2.882E-05	6.350E-03	25	A335	0 0 0 0 0	
2.890E-05	6.368E-03	25	A335	0 0 0 0 0	
3.177E-05	7.000E-03	25	M127	1 0 0 0 0	

3551. $C_{15}H_{24}O$

Nonylphenol

RN: 25154523 **MP** (°C)**:**
MW: 220.36 **BP** (°C)**:** 293–297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.224E-05	4.900E-03	25	B420	1 1 1 1 1	

3552. $C_{15}H_{26}N_2$

Sparteine
(–)-Spartein

RN: 90-39-1 **MP** (°C)**:** 30
MW: 234.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.297E-02	3.040E+00	22	F300	1 0 0 0 2	
1.297E-02	3.040E+00	25	D004	0 0 0 0 0	

3553. $C_{15}H_{26}N_2O_3$

5-Allyl-5-methylhexylcarbinylbarbituric acid

RN: **MP** (°C)**:**
MW: 282.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	3.060E+00	ns	T003	0 0 0 0 2	

3554. $C_{15}H_{26}N_2O_3$

5-Ethyl-5-*n*-nonylbarbituric acid
5-Ethyl-5-nonylbarbiturate

RN: 64810-91-9 **MP** (°C)**:**
MW: 282.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	9.742E-02	25	M310	2 2 2 2 2	

3555. $C_{15}H_{26}O_6$

Tributyrin
Glyceryl tributyrate
Tributanoylglycerol
1,2,3-Propanetriyl tributyrate

RN: 60-01-5 **MP** (°C)**:** 173
MW: 302.37 **BP** (°C)**:** 287.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-04	9.999E-02	ns	F014	0 0 0 0 1	

3556. $C_{15}H_{28}O_4$
1,13-Tridecanedicarboxylic acid
1,15-Pentadecandioic acid
RN: 1460-18-0 **MP** (°C)**:**
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-03	3.500E-01	21	B040	1 0 1 1 1	*sic*

3557. $C_{15}H_{30}$
1-Pentadecene
RN: 13360-61-7 **MP** (°C)**:**
MW: 210.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E-09	3.740E-07	23	C332	0 0 0 0 0	

3558. $C_{15}H_{30}O_2$
Pentadecylic acid
Pentadecanoic acid
RN: 1002-84-2 **MP** (°C)**:** 52
MW: 242.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.135E-05	7.600E-03	0	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20.0	R001	1 1 1 1 1	
5.775E-05	1.400E-02	30	B136	1 0 2 1 1	
5.775E-05	1.400E-02	30.0	R001	1 1 1 1 1	
7.013E-05	1.700E-02	45	B136	1 0 2 1 1	
7.013E-05	1.700E-02	45.0	R001	1 1 1 1 1	
8.251E-05	2.000E-02	60	B136	1 0 2 1 1	
8.250E-05	2.000E-02	60.0	R001	1 1 1 1 1	
3.135E-05	7.600E-03	.0	R001	1 1 1 1 1	

3559. $C_{15}H_{30}O_3$
Dodecyl lactate
Propanoic acid, 2-hydroxy-, dodecyl ester
RN: 6283-92-7 **MP** (°C)**:**
MW: 258.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-04	1.000E-01	25	R006	2 2 0 1 0	

3560. $C_{15}H_{32}$

Pentadecane
n-Pentadecane
Pentadecane-d32
Pentadecane (*n*)

RN: 629-62-9 **MP** (°C)**:** 9.9
MW: 212.42 **BP** (°C)**:** 270.63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.883E-10	4.000E-08	25	T423	0 0 0 0 0	

3561. $C_{15}H_{32}O$

Pentadecanol
Pentadecan-1-ol
1-Pentadecanol

RN: 629-76-5 **MP** (°C)**:** 46
MW: 228.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-07	1.028E-04	25	R002	0 0 0 0 0	

3562. $C_{16}H_8Cl_2F_6N_2O_3$

Hexaflumuron

RN: 86479-06-3 **MP** (°C)**:**
MW: 461.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-08	1.620E-05	20	M402	0 0 0 0 0	

3563. $C_{16}H_{10}$

Fluoranthene
1,2-Benzacenaphthene
1,2-(1,8-Naphthalenediyl)benzene
Benzo[j,k]fluorene
Idryl
FA

RN: 206-44-0 **MP** (°C)**:** 107
MW: 202.26 **BP** (°C)**:** 384

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-07	8.191E-05	8.10	M082	1 1 1 2 2	
4.050E-07	8.191E-05	8.10	M151	2 1 2 2 2	
4.058E-07	8.207E-05	8.14	M183	1 1 1 1 2	
5.290E-07	1.070E-04	13.20	M082	1 1 1 2 2	
5.290E-07	1.070E-04	13.20	M151	2 1 2 2 2	

(*continued*)

3563. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.295E-07	1.071E-04	13.24	M183	1 1 1 1 2	
7.330E-07	1.483E-04	19.70	M082	1 1 1 2 2	
7.330E-07	1.483E-04	19.70	M151	2 1 2 2 2	
7.339E-07	1.484E-04	19.74	M183	1 2 1 1 2	
1.190E-06	2.407E-04	20	E009	1 0 0 1 2	
9.394E-07	1.900E-04	20	H300	1 1 2 2 1	
8.850E-07	1.790E-04	20	V416	0 0 0 0 0	
5.933E-07	1.200E-04	24	H116	2 1 0 0 2	
1.000E-06	2.023E-04	24.60	M082	1 1 1 2 2	
1.000E-06	2.023E-04	24.60	M151	2 1 2 2 2	
1.003E-06	2.028E-04	24.64	M183	1 2 1 1 2	
1.400E-06	2.832E-04	25	A325	2 1 2 2 1	
1.023E-06	2.070E-04	25	D406	1 2 2 2 2	
1.320E-06	2.670E-04	25	K001	2 2 2 2 2	
1.335E-06	2.700E-04	25	L332	1 1 1 1 2	
1.285E-06	2.600E-04	25	M064	1 1 2 2 1	
1.019E-06	2.060E-04	25	M071	2 2 2 2 2	
1.300E-06	2.629E-04	25	M342	1 0 1 1 1	
1.167E-06	2.360E-04	25	S227	1 2 1 1 2	
1.019E-06	2.060E-04	25.00	M151	2 1 1 2 2	
1.187E-06	2.400E-04	27	D003	1 0 0 1 1	
1.305E-06	2.640E-04	29	M071	2 2 2 2 2	
1.305E-06	2.640E-04	29.00	M151	2 1 1 2 2	
1.380E-06	2.791E-04	29.90	M082	1 1 1 2 2	
1.380E-06	2.791E-04	29.90	M151	2 1 2 2 2	
1.382E-06	2.796E-04	29.94	M183	1 2 1 1 2	
2.947E-06	5.960E-04	40	V416	0 0 0 0 0	
8.464E-06	1.712E-03	60	V416	0 0 0 0 0	
1.300E-06	2.630E-04	ns	I332	0 0 0 0 1	

3564. $C_{16}H_{10}$

Pyrene

Benzo[def]phenanthrene

RN: 129-00-0 **MP** (°C)**:** 156

MW: 202.26 **BP** (°C)**:** 404

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-07	<2.02E-05	4	K049	1 2 1 1 0	
2.430E-07	4.915E-05	4.70	M082	1 1 1 2 2	
2.430E-07	4.915E-05	4.70	M151	2 1 2 2 2	
2.434E-07	4.924E-05	4.74	M183	1 2 1 1 2	
2.890E-07	5.845E-05	9.50	M082	1 1 1 2 2	
2.890E-07	5.845E-05	9.50	M151	2 1 2 2 2	
2.895E-07	5.855E-05	9.54	M183	1 2 1 1 2	
3.560E-07	7.200E-05	14.30	M082	1 1 1 2 2	
3.560E-07	7.200E-05	14.30	M151	2 1 2 2 2	
3.563E-07	7.206E-05	14.34	M183	1 2 1 1 2	

(*continued*)

3564. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-07	7.258E-05	15	B385	0 0 0 0 0	
4.610E-07	9.324E-05	18.70	M082	1 1 1 2 2	
4.610E-07	9.324E-05	18.70	M151	2 1 2 2 2	
4.617E-07	9.338E-05	18.74	M183	1 2 1 1 2	
5.200E-07	1.052E-04	20	E009	1 0 0 0 1	
5.200E-07	1.052E-04	20	E025	1 0 1 2 1	
4.700E-07	9.506E-05	20	H306	1 0 1 2 1	
5.370E-07	1.086E-04	21.20	M082	1 1 1 2 2	
5.370E-07	1.086E-04	21.20	M151	2 1 2 2 2	
5.394E-07	1.091E-04	21.24	M183	1 2 1 1 2	
7.200E-07	1.456E-04	22	A413	2 0 2 2 1	
6.279E-07	1.270E-04	22.20	W003	2 1 2 2 2	average of 3
6.675E-07	1.350E-04	24	H106	1 0 2 2 2	
1.582E-07	3.200E-05	24	H116	2 1 0 0 1	
6.675E-07	1.350E-04	24	M129	1 2 1 1 2	
5.834E-07	1.180E-04	25	B319	2 0 1 2 2	
6.490E-07	1.313E-04	25	B385	0 0 0 0 0	
7.700E-07	1.557E-04	25	K001	1 0 2 1 2	
4.700E-07	9.506E-05	25	K123	1 0 2 2 1	
7.911E-07	1.600E-04	25	L332	1 1 1 1 2	
6.675E-07	1.350E-04	25	M064	1 1 2 2 2	
6.526E-07	1.320E-04	25	M071	2 2 2 2 2	
6.675E-07	1.350E-04	25	M156	1 2 1 1 2	
6.670E-07	1.349E-04	25	M342	1 0 1 1 2	
3.955E-07	8.000E-05	25	P340	0 0 0 0 0	
3.556E-08	7.191E-06	25	R084	2 2 2 2 1	*sic*
7.400E-07	1.497E-04	25	R302	1 2 1 2 1	
8.455E-07	1.710E-04	25	S227	1 2 1 1 2	
6.526E-07	1.320E-04	25.00	M151	2 1 1 2 2	
6.730E-07	1.361E-04	25.50	M082	1 1 1 2 2	
6.730E-07	1.361E-04	25.50	M151	2 1 2 2 2	
6.728E-07	1.361E-04	25.54	M183	1 2 1 1 2	
8.158E-07	1.650E-04	27	D003	1 0 0 1 1	
8.010E-07	1.620E-04	29	M071	2 2 2 2 2	
8.010E-07	1.620E-04	29.00	M151	2 1 1 2 2	
8.390E-07	1.697E-04	29.90	M082	1 1 1 2 2	
8.390E-07	1.697E-04	29.90	M151	2 1 2 2 2	
8.411E-07	1.701E-04	29.94	M183	1 2 1 1 2	
1.147E-06	2.320E-04	34.50	W003	2 1 2 2 2	average of 2
9.888E-07	2.000E-04	35	B385	0 0 0 0 0	
1.973E-06	3.990E-04	44.70	W003	2 1 2 2 2	average of 3
2.784E-06	5.630E-04	50.10	W003	2 1 2 2 2	average of 3
3.758E-06	7.600E-04	55.60	W003	2 1 2 2 1	average of 3
3.659E-06	7.400E-04	56.00	W003	2 1 2 2 1	
4.648E-06	9.400E-04	60.70	W003	2 1 2 2 1	average of 3
6.329E-06	1.280E-03	65.20	W003	2 1 2 2 2	average of 2
9.196E-06	1.860E-03	71.90	W003	2 1 2 2 2	average of 3
1.093E-05	2.210E-03	74.70	W003	2 1 2 2 2	
6.675E-07	1.350E-04	ns	H123	0 0 0 0 0	

(*continued*)

3564. $C_{16}H_{10}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.675E-07	1.350E-04	ns	K304	0 0 0 0 2	
6.675E-07	1.350E-04	ns	M344	0 0 0 0 2	
5.000E-07	1.011E-04	ns	M383	0 2 1 1 0	
1.000E-06	2.023E-04	ns	W005	0 0 1 2 0	

3565. $C_{16}H_{10}N_2O_8S_2$

C.I. Acid blue 74(free acid)
Indigo-disulfosaeure-(5,5′)
Indigotinsulfonic acid
RN: 860-22-0 **MP** (°C)**:**
MW: 422.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.37E-02	~1.00E+01	25	F300	1 0 0 0 0	

3566. $C_{16}H_{11}NO_2$

Cinchophen
2-Phenyl-4-quinolinecarboxylic acid
2-Phenylcinchoninic acid
RN: 132-60-5 **MP** (°C)**:** 213
MW: 249.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-04	1.600E-01	25	L074	2 2 1 1 2	

3567. $C_{16}H_{12}F_3NO$

6H-Dibenz[b,e]azepin-6-one, 5,11-dihydro-5-(2,2,2-trifluoroethyl)-
RN: 155206-49-8 **MP** (°C)**:**
MW: 291.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.589E-05	4.627E-03	ns	M381	0 1 1 1 2	pH 7.0

3568. $C_{16}H_{12}N_2O_3$

5,5-Diphenylbarbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diphenyl
Barbituric acid, 5,5-diphenyl
5,5-Diphenylbarbiturate
RN: 21914-07-8 **MP** (°C)**:**
MW: 280.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-05	1.785E-02	25	P350	0 0 0 0 0	intrinsic

3569. $C_{16}H_{12}N_2O_4S$

Sulfanaphthoquinone

RN: **MP** (°C)**:**
MW: 328.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	4.500E-02	20	F073	1 2 2 2 1	

3570. $C_{16}H_{12}O_6$

Hematein
Haematein
Benz[b]indeno[1,2-d]pyran-9(6H)-one, 6α,7-dihydro-3,4,6α,10-tetrahydroxy-

RN: 475-25-2 **MP** (°C)**:** >200
MW: 300.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	6.000E-01	20	F300	1 0 0 0 1	

3571. $C_{16}H_{12}O_6$

Benzoic acid, 2-(acetyloxy)-, 2-carboxyphenyl ester

RN: 530-75-6 **MP** (°C)**:** 166.5
MW: 300.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.661E-05	2.000E-02	21	N335	0 0 0 0 0	

3572. $C_{16}H_{13}ClN_2O$

Diazepam
7-Chloro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
Valium
Valrelease
Vazepam
Diazemuls

RN: 439-14-5 **MP** (°C)**:** 125
MW: 284.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-04	4.200E-02	20	N059	2 0 2 2 2	average of 2
1.756E-04	5.000E-02	25	G084	2 0 2 2 1	
1.756E-04	5.000E-02	25	G095	2 1 2 2 1	
1.756E-04	5.000E-02	25	M159	1 0 2 2 0	EFG, pH 7.0
2.320E-04	6.606E-02	25	M320	2 2 1 1 2	
1.089E-04	3.100E-02	25	M457	0 0 0 0 0	
1.510E-04	4.300E-02	25	N055	2 0 2 2 1	
1.580E-04	4.500E-02	25	N055	2 0 2 1 2	

(*continued*)

3572. $C_{16}H_{13}ClN_2O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.721E-04	4.900E-02	25	N055	2 0 2 1 2	
1.405E-04	4.000E-02	30	R081	1 2 2 2 0	
2.900E-04	8.258E-02	50	M335	1 0 2 1 2	pH 6.0
1.200E-04	3.417E-02	ns	F327	0 0 1 2 2	
3.512E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.756E-04	5.000E-02	ns	M036	0 0 0 0 0	

3573. $C_{16}H_{13}Cl_2NO_4$

Aceclofenac

RN: 89796-99-6 **MP** (°C)**:**

MW: 354.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.034E-05	3.200E-02	32	C411	2 1 1 2 1	

3574. $C_{16}H_{13}I_3N_2O_3$

Iobenzamic acid

N-(3-Amino-2,4,6-triiodobenzoyl)-*N*-phenyl-β-alanine

Orbil

Osbiland

Razebil

Osbil

RN: 3115-05-7 **MP** (°C)**:**

MW: 662.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	1.150E-01	ns	H055	0 0 0 0 0	

3575. $C_{16}H_{13}NO_3$

C.I. Disperse red 3

N-(2-Hydroxyethyl)-1-aminoanthraquinone

Disperse red 3

Disperse red 66

RN: 4465-58-1 **MP** (°C)**:** 168

MW: 267.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	4.277E-03	25	B333	0 0 0 0 0	

3576. $C_{16}H_{13}N_3$

Yellow AB
1-Phenylazo-2-naphthylamine
RN: 85-84-7 **MP** (°C)**:** 102
MW: 247.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.213E-06	3.000E-04	37	H120	1 1 1 1 0	normal saline

3577. $C_{16}H_{13}N_3O_3$

Mebendazole
Methyl 5-benzoyl benzimidazole-2-carbamate
Pantelmin
Methyl 5-benzoyl-2-benzimidazolecarbamate
RN: 31431-39-7 **MP** (°C)**:** 288.5
MW: 295.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-06	5.000E-04	21	N337	0 0 0 0 0	pH 5
1.700E-06	5.020E-04	21	N337	0 0 0 0 0	pH 5
1.199E-04	3.540E-02	25	H075	1 0 2 1 2	polymorph C
2.414E-04	7.130E-02	25	H075	1 0 2 1 2	polymorph B
3.332E-05	9.840E-03	25	H075	1 0 2 1 2	polymorph A
3.725E-06	1.100E-03	288.5	D426	0 0 0 0 0	
1.318E-04	3.893E-02	ns	R427	0 0 0 0 0	

3578. $C_{16}H_{14}$

9,10-Dimethylanthracene
RN: 781-43-1 **MP** (°C)**:** 182
MW: 206.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-07	5.600E-05	25	M064	1 1 2 2 1	
2.700E-07	5.570E-05	25	M342	1 0 1 1 1	
2.715E-07	5.600E-05	ns	M344	0 0 0 0 2	

3579. $C_{16}H_{14}ClN_3O$

Chlordiazepoxide
7-Chloro-2-(methylamino)-5-phenyl-3H-1,4-benzodiazepine-4-oxide
Librium
Menrium
Tropium
SK-Lygen

RN: 58-25-3 **MP** (°C)**:** 236
MW: 299.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.607E-03	1.981E+00	ns	R427	0 0 0 0 0	
6.672E-03	2.000E+00	rt	M035	0 0 0 0 0	

3580. $C_{16}H_{14}Cl_2N_2O_2$

Phenobenzuron
Benzoyl-1-(3,4-dichlorophenyl)-3,3-dimethylurea
Benzomarc
Urea, *N*-benzoyl-*N*-(3,4-dichlorophenyl)-*N′*,*N′*-dimethyl-

RN: 3134-12-1 **MP** (°C)**:** 119
MW: 337.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.745E-05	1.600E-02	22	M161	1 0 0 0 1	

3581. $C_{16}H_{14}Cl_2O_3$

Chlorobenzilate
Ethyl 4,4′-dichlorobenzilate
Acaraben
Benzilen
Folbex
Kopmite

RN: 510-15-6 **MP** (°C)**:** 36
MW: 325.19 **BP** (°C)**:** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.998E-05	1.300E-02	20	F311	1 2 2 2 1	

3582. $C_{16}H_{14}Cl_2O_4$

Diclotop-methyl
Methyl (+/–)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate

RN: 51338-27-3 **MP** (°C)**:** 40
MW: 341.19 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.465E-04	5.000E-02	22	M161	1 0 0 0 1	

3583. $C_{16}H_{14}FNO$

6H-Dibenz[b,e]azepin-6-one, 5-(2-fluoroethyl)-5,11-dihydro-

RN: 155206-48-7 **MP** (°C)**:**
MW: 255.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.917E-04	7.448E-02	ns	M381	0 1 1 1 2	pH 7.0

3584. $C_{16}H_{14}N_2O$

Methaqualone
Quaalude
Mandrax
Somnafac

RN: 72-44-6 **MP** (°C)**:** 114–117
MW: 250.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-03	2.999E-01	23	P094	0 0 0 0 0	

3585. $C_{16}H_{14}N_2O_2$

C.I. Disperse blue 14
9,10-Anthracenedione, 1,4-bis(methylamino)-

RN: 2475-44-7 **MP** (°C)**:** 226
MW: 266.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-07	3.728E-05	25	B333	0 0 0 0 0	

3586. $C_{16}H_{14}N_2O_3$

3-(Hydroxymethyl)phenytoin
3-(Hydroxymethyl)-5,5-diphenyl-2,4-imidazolidinedione

RN: 21616-46-6 **MP** (°C)**:**
MW: 282.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.959E-04	1.400E-01	22	B154	1 1 1 1 1	0.1M HCl

3587. $C_{16}H_{14}N_2O_4$

C.I. Disperse blue 26
9,10-Anthracenedione, 1,5-dihydroxy-4,8-bis(methylamino)-
Resiren blue TG
Navilene blue GL
PTB 31

RN: 3860-63-7 **MP** (°C)**:** 217
MW: 298.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-08	2.028E-05	25	B333	0 0 0 0 0	

3588. $C_{16}H_{14}O_3$

Ketoprofen
2-(*meta*-Benzoylphenyl) propionic acid
Orudis
Alrheumat
Oruvail

RN: 22071-15-4 **MP** (°C)**:** 94
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.509E-04	6.380E-02	5	F306	1 0 1 2 2	intrinsic
9.045E-04	2.300E-01	21	B331	1 2 2 1 1	pH 7.4
3.696E-04	9.399E-02	22.5	B422	2 0 2 2 2	
4.640E-04	1.180E-01	25	A408	2 0 1 2 0	int
2.006E-04	5.100E-02	25	A427	0 0 0 0 0	
5.646E-04	1.436E-01	25	F306	1 0 1 2 2	intrinsic
1.156E-03	2.939E-01	32	C411	2 1 1 2 1	
8.066E-04	2.051E-01	37	F306	1 0 1 2 2	intrinsic
5.112E-04	1.300E-01	37	Y421	0 0 0 0 0	
3.933E-05	1.000E-02	amb	L434	0 0 0 0 0	
2.006E-04	5.100E-02	rt	H302	0 0 2 1 2	intrinsic
8.219E-04	2.090E-01	rt	R431	0 0 0 0 0	Average

3589. $C_{16}H_{14}O_3$

Fenbufen
3-(4-Biphenylylcarbonyl) propionic acid
Lederfen

RN: 36330-85-5 **MP** (°C)**:** 185
MW: 254.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-06	9.409E-04	5	F306	1 0 1 2 2	intrinsic
1.000E-05	2.543E-03	24.99	K447	0 0 0 0 0	pH 2.0
6.430E-05	1.635E-02	25	C314	0 0 0 0 0	
6.410E-05	1.630E-02	25	C314	0 0 0 0 0	
8.700E-06	2.212E-03	25	F301	1 1 0 0 1	pH 2.0, *sic*

(*continued*)

3589. $C_{16}H_{14}O_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-06	2.212E-03	25	F306	1 0 1 2 2	intrinsic
1.800E-05	4.577E-03	37	F306	1 0 1 2 2	intrinsic
7.865E-06	2.000E-03	rt	H302	0 0 2 1 1	intrinsic

3590. $C_{16}H_{15}ClN_2$

Medazepam
7-Chloro-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepine
Nobrium
RN: 2898-12-6 **MP** (°C)**:**
MW: 270.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.083E-02	37	L011	1 0 2 1 1	

3591. $C_{16}H_{15}Cl_2NO_2$

Clomeprop
2-(2,4-Dichloro-3-methylphenoxy)-*N*-phenylpropanamide
RN: 84496-56-0 **MP** (°C)**:**
MW: 324.21 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-08	3.168E-05	ns	R427	0 0 0 0 0	

3592. $C_{16}H_{15}Cl_3OS_2$

2-(*p*-Methylthiophenyl)-2-(*p*-methylsulfinylphenyl)-1,1,1-trichloroethane
RN: 28463-05-0 **MP** (°C)**:** 133-136
MW: 393.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.174E-06	1.250E-03	ns	K117	0 1 2 1 1	

3593. $C_{16}H_{15}Cl_3O_2$

Methoxychlor
1,1′-(2,2,2-Trichloroethylidene)-bis[4-methoxybenzene]
Maralate
Methoxy DDT
Marlate
Chemform
RN: 72-43-5 **MP** (°C)**:** 82.5
MW: 345.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.786E-08	2.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.302E-07	4.500E-05	25	B083	2 2 1 2 1	particle size 5 µm

(*continued*)

3593. $C_{16}H_{15}Cl_3O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-07	5.000E-05	25	P085	0 0 0 0 0	
2.893E-07	1.000E-04	25	W025	1 0 2 2 2	
2.748E-07	9.500E-05	35	B083	2 2 1 2 1	particle size 5 µm
5.352E-07	1.850E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.794E-06	6.200E-04	ns	K117	0 1 2 1 1	
8.679E-09	3.000E-06	ns	K138	0 0 0 0 2	
2.314E-06	8.000E-04	ns	M110	0 0 0 0 0	EFG
1.794E-06	6.200E-04	ns	M138	0 1 0 0 1	
3.472E-07	1.200E-04	ns	M344	0 0 0 0 1	
2.089E-07	7.222E-05	ns	R427	0 0 0 0 0	

3594. $C_{16}H_{15}Cl_3O_2S_2$

2,2-bis(*p*-Methylsulfinylphenyl)-1,1,1-trichloroethane
2-(*p*-Methylsulfoxidephenyl)-1,1,1-trichloroethane
RN: 28396-87-4 **MP** (°C)**:** 150–153
MW: 409.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.077E-05	2.900E-02	ns	K117	0 1 2 1 1	

3595. $C_{16}H_{15}Cl_3O_4S_2$

2,2-bis(*p*-Methylsulfonylphenyl)-1,1,1-trichloroethane
RN: 30665-94-2 **MP** (°C)**:** 236.0
MW: 441.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.395E-06	1.500E-03	ns	K117	0 1 2 1 1	

3596. $C_{16}H_{15}Cl_3S_2$

2,2-*bis*-(*p*-Methylthiophenyl)-1,1,1-trichloroethane
RN: 19679-38-0 **MP** (°C)**:** 115-117
MW: 377.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E-06	5.700E-04	ns	K117	0 1 2 1 1	

3597. $C_{16}H_{15}FN_2O_5$

1-Butyryloxymethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1-Butyryloxymethyl-3-benzoyl-5-fluorouracil
RN: 97108-48-0 **MP** (°C)**:** 81–82
MW: 334.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.855E-04	6.200E-02	22	B321	0 0 0 0 0	pH 4.0

3598. $C_{16}H_{15}NO$

4-Cyano-4′-propyloxybiphenyl
3 COB
RN: 52709-86-1 **MP** (°C)**:**
MW: 237.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-07	2.136E-04	21	D300	2 2 1 1 2	

3599. $C_{16}H_{15}NO_2$

N-Butyl-1,8-naphthalimide
Naphthalimide, *N*-butyl-
1H-Benz[de]isoquinoline-1,3(2H)-dione, 2-butyl-
RN: 6914-62-1 **MP** (°C)**:** 95
MW: 253.30 **BP** (°C)**:** 412.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	5.066E-03	23	B410	2 1 2 2 2	

3600. $C_{16}H_{15}NO_2$

Cinnamyl anthranilate
2-Propen-1-ol, 3-phenyl-, 2-aminobenzoate
2-Aminobenzoic acid 3-phenyl-2-propenyl ester
3-Phenyl-2-propen-1-yl anthranilate
3-Phenyl-2-propenyl 2-aminobenzoate
Cinnamyl alcohol
RN: 87-29-6 **MP** (°C)**:** 60
MW: 253.30 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.080E-07	2.300E-04	ns	B338	0 0 0 0 1	

3601. $C_{16}H_{15}NO_3$

Benzoylphenylalanine
N-Benzoyl-DL-phenylalanine
RN: 2901-76-0 **MP** (°C)**:**
MW: 269.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.156E-03	8.500E-01	25.1	N026	0 0 0 0 0	

3602. $C_{16}H_{15}NO_4$
Benzoyltyrosine
N-Benzoyl-L-tyrosine
RN: 2566-23-6 **MP** (°C)**:**
MW: 285.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.680E+00	25.1	N026	0 0 0 0 0	

3603. $C_{16}H_{15}N_5$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-nitrile, 11-cyclopropyl-5,11-dihydro-4-methyl
RN: **MP** (°C)**:**
MW: 277.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-05	5.035E-03	ns	M381	0 1 1 1 2	pH 7.0

3604. $C_{16}H_{15}N_5O_4S$
2,5-Disulfanilamidopyridine
RN: **MP** (°C)**:**
MW: 373.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-03	4.950E-01	37	R058	1 2 1 1 2	

3605. $C_{16}H_{16}$
1,2,3,6,7,8-Hexahydropyrene
RN: 1732-13-4 **MP** (°C)**:** 133
MW: 208.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	2.291E-04	4	K049	1 0 2 1 1	

3606. $C_{16}H_{16}ClN_3O_3S$
Metolazone
2-Methyl-3-(*o*-tolyl)-6-sulfamyl-7-chloro-1,2,3,4-tetrahydro-4-quinazolinone
Zaroxolyn
Mykrox
Diulo
RN: 17560-51-9 **MP** (°C)**:** 256.0
MW: 365.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.321E-05	3.410E-02	10	B030	1 0 1 1 2	
1.339E-04	4.900E-02	20	B030	1 0 1 1 2	

(*continued*)

3606. $C_{16}H_{16}ClN_3O_3S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-04	6.030E-02	25	B030	1 0 1 1 2	
1.971E-04	7.210E-02	30	B030	1 0 1 1 2	
2.236E-04	8.180E-02	35	B030	1 0 1 1 2	
2.733E-04	1.000E-01	36	B030	1 0 1 1 2	
1.640E-04	6.000E-02	37	H013	1 0 0 0 0	
2.952E-04	1.080E-01	40	B030	1 0 1 1 2	
3.799E-04	1.390E-01	45	B030	1 0 1 1 2	
4.155E-04	1.520E-01	50	B030	1 0 1 1 2	

3607. $C_{16}H_{16}N_2$

3,4,7,8-Tetramethyl-1,10-phenanthroline

RN: 1660-93-1 **MP** (°C)**:** 278.5
MW: 236.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-06	1.512E-03	25.04	B094	1 2 1 2 1	

3608. $C_{16}H_{16}N_2O_4$

Phenmedipham

Methyl *m*-hydroxycarbanilate *m*-methylcarbanilate

RN: 13684-63-4 **MP** (°C)**:** 143
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.33E-05	<1.00E-02	20	B200	1 0 0 0 0	
3.330E-06	1.000E-03	20	F311	1 2 2 2 1	
1.397E-05	4.194E-03	25	H434	0 0 0 0 0	
3.330E-05	1.000E-02	ns	M061	0 0 0 0 1	
9.989E-06	3.000E-03	rt	M161	0 0 0 0 0	

3609. $C_{16}H_{16}N_2O_4$

Desmedipham

Ethyl *m*-hydroxycarbanilate carbanilate

Carbamic acid, *N*-phenyl-, 3-((ethoxycarbonyl)amino)phenyl ester

Betanex

Betanal-475

Betamix 70 WP

RN: 13684-56-5 **MP** (°C)**:** 120
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-05	7.000E-03	rt	M161	0 0 0 0 0	
2.331E-05	7.000E-03	rt	R304	0 0 0 0 0	

3610. $C_{16}H_{16}N_4$
Disperse black 1
RN: 6054-48-4 **MP** (°C)**:**
MW: 264.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-07	7.930E-05	25	B333	0 0 0 0 0	

3611. $C_{16}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′3′-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-2,4-dimethyl-
RN: 135794-77-3 **MP** (°C)**:**
MW: 280.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.346E-05	1.499E-02	ns	M381	0 1 1 1 2	pH 7.0

3612. $C_{16}H_{16}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-cyclobutyl-5,11-dihydro-5-methyl-
RN: 135794-88-6 **MP** (°C)**:**
MW: 280.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.911E-04	8.160E-02	ns	M381	0 1 1 1 2	pH 7.0

3613. $C_{16}H_{16}N_6O_4S$
2,5-Disulfanilamidopyrimidine
RN: **MP** (°C)**:**
MW: 388.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.664E-05	2.200E-02	37	R046	1 2 1 1 1	

3614. $C_{16}H_{16}O_2$
4-Methoxy-3,3′-dimethylbenzophenone
RN: 41295-28-7 **MP** (°C)**:** 62.25
MW: 240.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.323E-06	2.000E-03	20	M161	1 0 0 0 0	

3615. $C_{16}H_{16}O_3$

Ethyl benzoyl benzoate

RN: 106396-19-4 **MP** (°C)**:**
MW: 256.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.901E-04	9.999E-02	ns	F014	0 0 0 0 1	

3616. $C_{16}H_{16}O_3$

Anisyl phenylacetate
p-Methoxybenzyl phenylacetate
Phenylacetic acid, *p*-methoxybenzyl ester

RN: 102-17-0 **MP** (°C)**:**
MW: 256.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	5.126E-01	25	D407	1 0 2 2 2	
2.000E-03	5.126E-01	ns	S460	0 0 0 0 0	

3617. $C_{16}H_{17}ClN_2S$

Chlorphenethazine
2-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-ethanamide

RN: 2095-24-1 **MP** (°C)**:**
MW: 304.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-05	4.573E-03	ns	G023	0 0 1 1 1	

3618. $C_{16}H_{17}ClN_4O_3$

C.I. Disperse red 13
4-Nitro-2-chloro-4′-[ethyl(2-hydroxyethyl)amino]azobenzene
Acetoquinone light rubine BLZ
Acetamine rubine B
Acetate fast rubine B

RN: 3180-81-2 **MP** (°C)**:** 133
MW: 348.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-08	1.151E-05	25	B333	0 0 0 0 0	

3619. $C_{16}H_{17}ClN_4O_4$

C.I. Disperse red 7
Ethanol, 2,2′-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]*bis*-
RN: 4540-00-5 **MP** (°C)**:** 190
MW: 364.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.013E-04	25	B333	0 0 0 0 0	

3620. $C_{16}H_{17}NO$

Diphenamid
Dyamid
Enide
N,N-Dimethyl-α-phenylbenzeneacetamide
N,N-Dimethyldiphenylacetamide
Diherbid
RN: 957-51-7 **MP** (°C)**:** 132
MW: 239.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	2.399E-01	25	M061	1 0 0 0 1	
1.086E-03	2.600E-01	25	M161	1 0 0 0 2	
1.090E-03	2.609E-01	27	B200	1 0 0 0 2	
1.086E-03	2.600E-01	ns	B185	0 0 0 0 0	
2.079E-02	4.975E+00	ns	B200	0 0 0 0 0	
1.086E-03	2.600E-01	ns	H042	0 0 0 0 2	

3621. $C_{16}H_{17}NO_4$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-amino-2-oxoethyl ester, (*S*)
Naproxen, *N,N*-glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-amino-2-oxoethyl ester
Naproxen *N,N*-glycolamide ester
RN: 114665-17-7 **MP** (°C)**:** 139.5
MW: 287.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.183E-04	3.400E-02	21	B331	1 2 2 1 2	pH 7.4
1.183E-04	3.400E-02	21	B331	0 0 0 0 0	

3622. $C_{16}H_{17}N_3O_4S$
Cephalexin
Cefanex
C-Lexin
Keflex
Cefalexin
RN: 15686-71-2 **MP** (°C)**:**
MW: 347.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.724E-02	5.990E+00	10	O305	2 2 1 2 2	noncrystalline
1.569E-01	5.450E+01	15	O305	2 2 1 2 2	noncrystalline
1.416E-01	4.920E+01	20	O305	2 2 1 2 2	noncrystalline
3.598E-02	1.250E+01	25	P311	0 0 0 0 0	EFG
1.330E-02	4.620E+00	25	U001	0 0 0 0 0	
3.500E-03	1.216E+00	35	E311	0 0 0 0 0	

3623. $C_{16}H_{17}N_3O_4S.H_2O$
Cephalexin (monohydrate)
RN: 23325-78-2 **MP** (°C)**:**
MW: 365.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.694E-02	1.350E+01	25	M165	1 0 0 0 2	

3624. $C_{16}H_{17}N_5O_5$
Dis. A. 12
Ethanol, 2-[[4-[(2,4-dinitrophenyl)azo]phenyl]ethylamino]-
RN: 62570-20-1 **MP** (°C)**:**
MW: 359.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	7.187E-04	25	B333	0 0 0 0 0	

3625. $C_{16}H_{17}N_5O_6$
Dis. A. 14
4-[bis(2-Hydroxyethyl)amino]-2′,4′-dinitroazobenzene
RN: 60129-67-1 **MP** (°C)**:**
MW: 375.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	2.252E-03	25	B333	0 0 0 0 0	

3626. $C_{16}H_{18}ClNO_4S$

Oxathiin carboxanilide

Benzoic acid, 2-chlloro-5-[[(5,6-dihydro-2-methyl-1,4-oxathiin-3-yl)carnonyl]amino]isopropyl Ester

RN: 135812-04-3 **MP** (°C)**:** 130

MW: 355.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.653E-06	1.300E-03	25	O319	0 0 0 0 0	

3627. $C_{16}H_{18}FN_3O_3$

Norfloxacin

Noroxin

RN: 70458-96-7 **MP** (°C)**:**

MW: 319.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-04	2.700E-01	6	Y421	0 0 0 0 0	
6.576E-04	2.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
6.263E-04	2.000E-01	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer
2.505E-02	8.000E+00	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
5.950E-04	1.900E-01	25	A414	1 0 1 1 1	
1.159E-03	3.700E-01	25	Y421	0 0 0 0 0	
2.662E-03	8.500E-01	40	Y421	0 0 0 0 0	

3628. $C_{16}H_{18}NO_5P$

Diphenylmorpholidophosphate

RN: **MP** (°C)**:**

MW: 335.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.844E-03	2.295E+00	25	A040	1 0 0 0 2	

3629. $C_{16}H_{18}N_2O_3$

Difenoxuron

N-4-(4′-Methoxyphenoxy)phenyl-*N′*,*N′*-dimethylurea

C-3470

RN: 14214-32-5 **MP** (°C)**:** 138.5

MW: 286.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.985E-05	2.000E-02	20	M161	1 0 0 0 1	
6.985E-05	2.000E-02	ns	M061	0 0 0 0 1	

3630. $C_{16}H_{18}N_2O_4S$
Penicillin G
Benzylpenicillin
Pfizerpen
RN: 61-33-6 **MP** (°C)**:**
MW: 334.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	2.675E+00	25	U001	0 0 0 0 0	

3631. $C_{16}H_{18}N_4O$
6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-(1,1-dimethylethyl)-5,11-dihydro-5-methyl-
RN: 135794-80-8 **MP** (°C)**:**
MW: 282.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.416E-05	3.997E-03	ns	M381	0 1 1 1 2	pH 7.0

3632. $C_{16}H_{18}N_4O_2$
Dye III
4[[(4-Diethylamino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 298.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-07	2.715E-04	97.40	B198	1 2 1 1 1	

3633. $C_{16}H_{18}N_4O_2$
Dis. A. 5
4-Nitro-4′-diethylaminoazobenzene
4-Nitro-4′-*N,N*-diethylaminoazobenzene
DEANAB
RN: 3025-52-3 **MP** (°C)**:** 152
MW: 298.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-11	1.193E-08	25	B333	0 0 0 0 0	

3634. $C_{16}H_{18}N_4O_3$

Disperse red 1
Dye IV
C.I. Disperse red 1
1-[*N*-Ethyl-*N*-(2-hydroxyethyl)amino]-4-(4-nitrophenylazo)benzene
4-Nitro-4′-[ethyl(2-hydroxyethyl)amino]azobenzene
RN: 2872-52-8 **MP** (°C)**:** 161
MW: 314.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-07	1.697E-04	25	B333	0 0 0 0 0	
5.400E-06	1.697E-03	60	B198	1 2 1 1 1	
6.521E-06	2.050E-03	60	P313	0 0 0 0 0	average of 2
1.082E-05	3.400E-03	70	P313	0 0 0 0 0	average of 2
1.310E-05	4.118E-03	71.80	B198	1 2 1 1 2	
1.797E-05	5.650E-03	80	P313	0 0 0 0 0	average of 2
3.120E-05	9.808E-03	84.10	B198	1 2 1 1 2	
3.388E-05	1.065E-02	90	P313	0 0 0 0 0	average of 2
7.130E-05	2.241E-02	97.40	B198	1 2 1 1 2	

3635. $C_{16}H_{18}N_4O_4$

Disperse red 19
Dye V
C.I. Disperse red 19
2-[(2-Hydroxyethyl)[4-(4-nitrophenylazo)phenyl]amino]ethanol
4′-[(*N,N*-Dihydroxyethyl)amino]-4-nitroazobenzene
RN: 2734-52-3 **MP** (°C)**:** 209
MW: 330.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-07	2.345E-04	25	B333	0 0 0 0 0	
1.170E-05	3.865E-03	60	B198	1 2 1 1 2	
3.030E-05	1.001E-02	71.80	B198	1 2 1 1 2	
8.330E-05	2.752E-02	84.10	B198	1 2 1 1 2	
2.100E-04	6.937E-02	97.40	B198	1 2 1 1 2	

3636. $C_{16}H_{18}O_3$

Naproxen ethyl esterv
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, ethyl ester, (alpha*S*)-
RN: 31220-35-6 **MP** (°C)**:**
MW: 258.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.645E-06	1.200E-03	21	B331	1 2 2 1 2	pH 7.4
4.645E-06	1.200E-03	21	B331	0 0 0 0 0	

3637. $C_{16}H_{19}ClN_2$

Chlorpheniramine
1-(*p*-Chlorophenyl)-1-(2-pyridyl)-3-dimethylaminopropane
RN: 132-22-9 **MP** (°C)**:** <25
MW: 274.80 **BP** (°C)**:** 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.496E+00	37.5	L034	2 2 0 1 2	pH 7.4

3638. $C_{16}H_{19}NO_7$

Benzoic acid, 2-(acetyloxy)-, 2-[(2-ethoxy-2-oxoethyl)methylamino]-2-oxoethyl ester
RN: 116482-77-0 **MP** (°C)**:** 47.5
MW: 337.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-03	9.600E-01	21	N335	0 0 0 0 0	

3639. $C_{16}H_{19}N_3O_2$

C.I. Solvent yellow 58
p-[bis(2-Hydroxyethyl)amino]azobenzene
4-[bis(2-Hydroxyethyl)amino]azobenzene
RN: 2452-84-8 **MP** (°C)**:** 134
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.139E-02	25	B333	0 0 0 0 0	

3640. $C_{16}H_{19}N_3O_4S$

Cephradine
Anspor
Velosef
RN: 38821-53-3 **MP** (°C)**:** 140
MW: 349.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-02	2.130E+01	ns	F181	0 0 0 0 2	

3641. $C_{16}H_{19}N_3O_4S$

Ampicillin
(2*S*,5*R*,6*R*)-6-[(*R*)-2-Amino-2-phenylacetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0] heptane-2-carboxylic acid
Aminobenzylpenicillin
Unasyn
Wymox
Totacillin

RN: 69-53-4 **MP** (°C)**:**
MW: 349.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.293E-02	1.500E+01	7.5	P009	1 0 2 1 0	EFG
3.721E-02	1.300E+01	20	P009	1 0 2 1 0	EFG
2.890E-02	1.010E+01	21	M044	2 0 2 2 2	
3.978E-02	1.390E+01	25	H051	1 2 2 2 2	
6.600E-03	2.306E+00	25	K444	0 0 0 0 0	
3.434E-02	1.200E+01	30	P009	1 0 2 1 0	EFG
3.291E-02	1.150E+01	40	P009	1 0 2 1 0	EFG

3642. $C_{16}H_{19}N_3O_4S.3H_2O$

Ampicillin (trihydrate)

RN: 7177-48-2 **MP** (°C)**:** 198
MW: 403.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-02	5.700E+00	7.5	P009	1 0 2 1 0	EFG
1.487E-02	6.000E+00	20	P009	1 0 2 1 0	EFG
1.873E-02	7.558E+00	21	M044	2 0 2 2 2	
1.983E-02	8.000E+00	30	P009	1 0 2 1 0	EFG
2.479E-02	1.000E+01	40	P009	1 0 2 1 0	EFG

3643. $C_{16}H_{19}N_3O_5S$

Amoxicillin

RN: 61336-70-7 **MP** (°C)**:**
MW: 365.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	4.000E+00	ns	K444	0 0 0 0 0	

3644. $C_{16}H_{19}N_3O_5S.3H_2O$

Amoxicillin (trihydrate)
4-Thia-1-azabicyclo(3,2,0)heptane-2-carboxylic acid (trihydrate)
RN: 61336-70-7 **MP** (°C)**:**
MW: 419.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.54E-03	~4.00E+00	ns	B188	0 0 0 0 0	

3645. $C_{16}H_{19}N_5O$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 2-dimethylamino)-11-ethyl-5,11-dihydro-4-methyl-
RN: 135795-08-3 **MP** (°C)**:**
MW: 297.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E-05	4.002E-03	ns	M381	0 1 1 1 2	pH 7.0

3646. $C_{16}H_{19}N_5O_2$

6H-Dipyrido[3,2-b:2′,3′-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-[(2-hydroxyethyl) methylamino
RN: 155206-46-5 **MP** (°C)**:**
MW: 313.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	1.368E-01	ns	M381	0 1 1 1 2	pH 7.0

3647. $C_{16}H_{19}O_4P$

Butyl diphenyl phosphate
RN: 2752-95-6 **MP** (°C)**:**
MW: 306.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3648. $C_{16}H_{20}I_3N_3O_7$

1,3-Benzenedicarboxamide, *N*-(2-hydroxyethyl)-*N′*-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-
RN: 77868-44-1 **MP** (°C)**:**
MW: 747.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.625E-02	1.961E+01	25	P091	0 0 0 0 0	

3649. $C_{16}H_{20}I_3N_3O_7$

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N′*-(2-hydroxyethyl)-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(*RS*)

RN: 77868-43-0 **MP** (°C)**:**
MW: 747.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.374E-02	4.762E+01	25	P091	0 0 0 0 0	

3650. $C_{16}H_{20}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(hydroxyacetyl)amino]-2,4,6-triiodo- [*RS*-(*RS**,*RS**)]-

RN: 77868-40-7 **MP** (°C)**:**
MW: 763.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.317E-02	1.768E+01	25	P091	0 0 0 0 0	

3651. $C_{16}H_{20}I_3N_3O_8$

1,3-Benzenedicarboxamide, 5-[(hydroxyacetyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 77868-41-8 **MP** (°C)**:**
MW: 763.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.282E-02	4.031E+01	25	P091	0 0 0 0 0	

3652. $C_{16}H_{20}N_4O_2$

Apazone
APZ
Azapropazone

RN: 13539-59-8 **MP** (°C)**:** 247
MW: 300.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.472E-01	35	H091	1 2 2 2 1	*sic*
2.896E-04	8.700E-02	rt	H302	0 0 2 1 1	intrinsic

3653. $C_{16}H_{20}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-isobutylpyrimidine

RN: **MP** (°C)**:**
MW: 348.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.091E-05	3.800E-03	37	R076	1 2 0 0 1	

3654. $C_{16}H_{20}N_8O_2S$

6-[D-2-Amino-2-(4-aminophenyl)-acetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3,2,0]hept-2-yl-5-t

RN: **MP** (°C)**:**
MW: 388.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.277E-03	2.050E+00	25	B148	2 2 2 1 2	

3655. $C_{16}H_{20}O_6P_2S_3$

Temephos
O,O′-(Thiodi-4,1-phenylene)bis(*O,O′*-dimethylphosphorothioate)
Abate
Tetramethyl *O,O′*-thiodi-*p*-phenylene phosphorothioate
Abaphos
Tetrafenphos

RN: 3383-96-8 **MP** (°C)**:**
MW: 466.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-08	9.000E-06	10	B324	0 0 0 0 0	
1.929E-08	8.998E-06	10	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B300	2 1 1 1 2	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
1.501E-06	7.002E-04	30	B324	0 0 0 0 0	
1.501E-06	7.000E-04	30	B324	0 0 0 0 0	

3656. $C_{16}H_{21}ClN_3S$

Methylene blue
Methylenblau
C.I. 52015

RN: 61-73-4 **MP** (°C)**:**
MW: 322.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.02E-01	~3.30E+01	20	F300	1 0 0 0 0	

3657. $C_{16}H_{21}NO$

N,N-Heptamethylenecinnamamide
Octahydro-1-(1-oxo-3-phenyl-2-propenyl) azocine

RN: 59832-06-3 **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	6.230E-02	ns	H350	0 0 0 0 0	

3658. $C_{16}H_{21}NO$

N-Cycloheptylcinnamamide
N-Cycloheptyl-3-phenyl-2-propenamide
RN: 59831-98-0 **MP** (°C)**:**
MW: 243.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-06	8.688E-04	ns	H350	0 0 0 0 0	

3659. $C_{16}H_{21}NO_2$

Propranolol
2-Propanol, 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-
RN: 525-66-6 **MP** (°C)**:**
MW: 259.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-04	3.100E-02	22.5	B422	0 0 0 0 0	
3.123E-04	8.099E-02	25	S450	0 0 0 0 0	
3.092E-08	8.020E-06	32	M458	0 0 0 0 0	

3660. $C_{16}H_{21}NO_2S$

m-Carboxyloctylphenylisothiocyanate
3-Carboxyloctylphenylisothiocyanate
RN: **MP** (°C)**:**
MW: 291.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.748E-02	25	K032	2 2 0 1 1	

3661. $C_{16}H_{21}NO_3$

Piperidine, 1-[(benzoyloxy)acetyl]-2-ethyl-
RN: 115178-69-3 **MP** (°C)**:** 54.5
MW: 275.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.889E-03	5.200E-01	22	N317	1 1 2 1 2	

3662. $C_{16}H_{21}NO_3$

Piperidine, 1-[(benzoyloxy)acetyl]-2,6-dimethyl-
RN: 115178-70-6 **MP** (°C)**:** 118
MW: 275.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.448E-04	1.500E-01	22	N317	1 1 2 1 2	

3663. $C_{16}H_{21}NO_3$

Acetamide, 2-(benzoyloxy)-*N*-cyclohexyl-*N*-methyl-

RN: 106231-65-6 **MP** (°C)**:**
MW: 275.35 **BP** (°C)**:** 439.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.084E-04	1.400E-01	22	B427	1 0 0 1 1	

3664. $C_{16}H_{21}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-(diethylamino)-1-methyl-2-oxoethyl ester

RN: 118247-09-9 **MP** (°C)**:** 40.5
MW: 307.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.499E-02	7.680E+00	21	N335	0 0 0 0 0	

3665. $C_{16}H_{21}N_3$

Tripelennamine
N-Benzyl-*N′*,*N′*-dimethyl-*N*-2-pyridylethylenediamine
PBZ
Pelamine

RN: 91-81-6 **MP** (°C)**:** <25
MW: 255.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	5.873E-01	30	L068	1 0 0 1 0	EFG
1.500E-02	3.830E+00	37.5	L034	2 2 0 1 2	pH 7.4

3666. $C_{16}H_{22}Cl_2O_3$

2,4-Dichlorophenoxyacetic acid *n*-octyl ester
2,4-Dichlorophenoxyacetic acid capryl ester

RN: 1928-44-5 **MP** (°C)**:**
MW: 333.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.128E-05	7.092E-03	ns	M120	0 0 1 1 2	

3667. $C_{16}H_{22}N_4O$

Neohetramine
N,N-Dimethyl-*N′*-(*p*-methoxybenzyl)-*N′*-(2-pyrimidyl)ethylenediamine
Tonzilamine
RN: 91-85-0 **MP** (°C)**:**
MW: 286.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	5.441E+00	37.5	L034	2 2 0 1 2	pH 7.4

3668. $C_{16}H_{22}N_4O_2S$

2-Sulfanilamido-4-methyl-5-*n*-amylpyrimidine
RN: 71119-35-2 **MP** (°C)**:** 188-190
MW: 334.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-05	2.800E-02	29	C049	0 0 0 0 0	

3669. $C_{16}H_{22}N_4O_6$

2′-Valeryl-6-methoxypurine arabinoside
2′-Trimethylacetyl-6-methoxypurine arabinoside
RN: 121032-22-2 **MP** (°C)**:** 118–120
MW: 366.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-01	8.793E+01	37	C348	0 0 0 0 0	pH 7.00
1.070E-01	3.920E+01	37	C348	0 0 0 0 0	pH 7.00

3670. $C_{16}H_{22}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-pivalate-β-D-arabinofuranosyl)]-9H-purine (hemihydrate)
RN: 121032-42-6 **MP** (°C)**:** glass
MW: 375.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-02	1.336E+01	37	M378	1 2 1 1 2	pH 7.2

3671. $C_{16}H_{22}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-valerate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 142963-77-7 **MP** (°C)**:** foam
MW: 375.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-03	6.457E-01	37	M378	1 2 1 1 2	pH 7.2

3672. $C_{16}H_{22}O_4$

Dibutyl phthalate
n-Butyl phthalate
RN: 84-74-2 **MP** (°C)**:** –35
MW: 278.35 **BP** (°C)**:** 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.455E-05	1.240E-02	10	S198	2 1 2 2 2	
3.952E-05	1.100E-02	15	H069	1 0 1 1 1	
3.630E-05	1.010E-02	20	L300	2 1 0 2 2	
3.880E-05	1.080E-02	20	S198	2 1 2 2 2	
3.593E-04	1.000E-01	22	N311	1 0 1 1 2	
3.377E-05	9.400E-03	22	Y419	0 0 0 0 0	
6.574E-05	1.830E-02	23.5	S171	2 1 2 2 2	
3.126E-05	8.700E-03	25	D336	0 0 0 0 0	
3.449E-05	9.600E-03	25	D336	0 0 0 0 0	
4.670E-05	1.300E-02	25	F067	1 0 2 2 2	
1.609E-02	4.480E+00	25	F070	1 0 0 0 2	*sic*
4.095E-05	1.140E-02	30	S198	2 1 2 2 2	
1.437E-03	4.000E-01	rt	M161	0 0 0 0 2	

3673. $C_{16}H_{22}O_4$

Diisobutyl phthalate
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) esterpalatinol
Phthalic acid diisobutyl ester
Palatinolic
RN: 84-69-5 **MP** (°C)**:**
MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.592E-04	9.999E-02	20	F070	1 0 0 0 2	
7.300E-05	2.032E-02	20	L300	2 1 0 2 2	
2.227E-05	6.200E-03	24	H116	2 1 0 0 2	
5.030E-06	1.400E-03	25	D336	0 0 0 0 0	

3674. $C_{16}H_{22}O_4$

tere-Butyl phthalate
RN: 30448-43-2 **MP** (°C)**:**
MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-06	1.100E-03	25	D336	0 0 0 0 0	

3675. $C_{16}H_{22}O_4$

Di-*n*-butyl *o*-phthalate

RN: **MP** (°C)**:** –35 C

MW: 278.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.593E-05	1.000E-02	25	S417	0 0 0 0 0	

3676. $C_{16}H_{22}O_6$

Diethoxyethyl phthalate

bis(2-Ethoxyethyl) phthalate

RN: 605-54-9 **MP** (°C)**:**

MW: 310.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.271E-03	1.946E+00	ns	F014	0 0 0 0 2	

3677. $C_{16}H_{22}O_8.2H_2O$

Coniferin (dihydrate)

4-Hydroxy-3-methoxy-1-(γ-hydroxypropenyl)benzene-4-D-glucoside (dihydrate)

Abietin(dihydrate)

Coniferosi(dihydrate)

RN: 531-29-3 **MP** (°C)**:** 185

MW: 378.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-02	4.975E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3678. $C_{16}H_{22}O_{11}$

β-D-Glucose pentaacetate

β-Glucose-penta-acetat

RN: 604-69-3 **MP** (°C)**:** 131

MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.306E-03	9.000E-01	18	F300	1 0 0 0 0	

3679. $C_{16}H_{22}O_{11}$

α-D-Glucose pentaacetate
1,2,3,4,6-Penta-*O*-acetyl-α-D-glucose
Pentaacetate
Glucopyranose pentaacetate
Glucose pentaacetate;
α-D-Glucopyranose

RN: 604-68-2 **MP** (°C)**:** 109–111
MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	1.484E+00	ns	R427	0 0 0 0 0	

3680. $C_{16}H_{22}O_{11}$

α-Glucose pentaacetate
α-Glucose-penta-acetat

RN: 3891-59-6 **MP** (°C)**:** 110
MW: 390.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.843E-03	1.500E+00	18	F300	1 0 0 0 1	

3681. $C_{16}H_{23}FN_2O_6$

1,3-bis(Pivaloyloxymethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one
1,3-bis(Pivaloyloxymethyl)-5-fluorouracil

RN: 66542-50-5 **MP** (°C)**:** 102–104
MW: 358.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.256E-04	4.500E-02	22	B321	0 0 0 0 0	pH 4.0

3682. $C_{16}H_{23}NO$

n-Heptylcinnamamide
2-Propenamide, *N*-heptyl-3-phenyl-

RN: 59831-99-1 **MP** (°C)**:**
MW: 245.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-06	1.865E-03	ns	H350	0 0 0 0 0	

3683. $C_{16}H_{23}NO_2$

Etoxadrol
(+)-2-(2-Ethyl-2-phenyl-1,3-dioxolan-4-yl)piperidine
RN: 28189-85-7 **MP** (°C)**:**
MW: 261.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-03	6.500E-01	20	K017	1 2 2 2 2	pH 10, intrinsic
1.098E-02	2.870E+00	30	K017	1 2 2 2 2	pH 10, intrinsic
4.668E-02	1.220E+01	40	K017	1 2 2 2 2	pH 10, intrinsic

3684. $C_{16}H_{23}NO_3$

Acetaminophen octanoate
Octanoic acid, 4-(acetylamino)phenyl ester
RN: 54942-41-5 **MP** (°C)**:** 103
MW: 277.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.605E-05	1.000E-02	25	B010	1 1 1 1 0	

3685. $C_{16}H_{23}NO_3S_2$

N-[2-(3,4-Dihydroxyphenyl)ethyl]-5-[(3*R*)-1,2-dithiolan-3-yl]-pentanamide
RN: **MP** (°C)**:**
MW: 341.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-06	3.600E-04	ns	S453	0 0 0 0 0	

3686. $C_{16}H_{23}NO_6$

Monocrotaline
(–)-Monocrotaline
RN: 315-22-0 **MP** (°C)**:** 202
MW: 325.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.644E-02	1.186E+01	ns	I312	0 0 0 0 0	

3687. $C_{16}H_{23}N_5O_5$

9-[5′-(*O*-Caproyl)-β-D-arabinofuranosyl]adenine ester
RN: 65926-34-3 **MP** (°C)**:**
MW: 365.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-03	2.500E+00	ns	B134	0 1 1 1 1	

3688. $C_{16}H_{23}N_5O_5$
9-[5′-(*O-tert*-Butylacetyl)-β-D-arabinofuranosyl]adenine ester
RN: 68325-42-8 **MP** (°C)**:**
MW: 365.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.135E-02	7.800E+00	ns	B134	0 1 1 1 1	

3689. $C_{16}H_{24}N_2O_2$
N,N,N′,N′-Tetraethylterephthalamide
RN: 15394-30-6 **MP** (°C)**:**
MW: 276.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.528E+00	30	K019	1 0 0 0 1	

3690. $C_{16}H_{24}N_2O_2$
N,N,N′,N′-Tetraethylisophthalamide
RN: 13698-87-8 **MP** (°C)**:**
MW: 276.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	1.990E+02	30	K019	1 0 0 0 2	

3691. $C_{16}H_{24}N_4O_2$
2,5-Diaziridinyl-3,6-bis(propylamino)-1,4-benzoquinone
RN: 59886-47-4 **MP** (°C)**:** 140
MW: 304.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.29E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3692. $C_{16}H_{24}N_4O_6$
2,5-Diaziridinyl-3,6-bis(2′-hydroxyl-3′-hydroxylpropylamino)-1,4-benzoquinone
2,5-Diaziridinyl-3,6-bis(hydroxylethylmethylamino)-1,4-benzoquinone
RN: 59886-55-4 **MP** (°C)**:** 273
MW: 368.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.629E-01	6.000E+01	rt	C317	0 0 0 0 0	
8.143E-02	3.000E+01	rt	C317	0 0 0 0 0	

3693. $C_{16}H_{24}N_6$

1-(Methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine

RN: 125867-93-8 **MP** (°C)**:**

MW: 300.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-05	7.291E-03	25	B386	0 0 0 0 0	

3694. $C_{16}H_{24}O_3$

Nonyl *p*-hydroxybenzoate

Nonyl 4-hydroxybenzoate

RN: 38713-56-3 **MP** (°C)**:**

MW: 264.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-03	1.275E+00	25	D081	1 2 2 1 2	

3695. $C_{16}H_{24}O_4$

3,4-Epoxy-6-methylcyclohexylmethyl-3,4-epoxy-6-methylcyclohexane carboxylate

EP 201

RN: 141-37-7 **MP** (°C)**:**

MW: 280.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E-02	2.991E+00	ns	I313	0 0 0 0 0	

3696. $C_{16}H_{25}NOS$

S-Benzyl di-*sec*-butylthiocarbamate

Thiocarbazil

Tiocarbazil

RN: 36756-79-3 **MP** (°C)**:**

MW: 279.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.946E-06	2.500E-03	30	M161	1 0 0 0 1	

3697. $C_{16}H_{25}NO_2$
Butacarb
Carbamic acid, *N*-methyl-, 3,5-di-*tert*-butylphenyl ester
3,5-Di-*tert*-butylphenyl methylcarbamate
RN: 2655-19-8 **MP** (°C)**:** 102.9
MW: 263.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.695E-05	1.500E-02	20	M161	1 0 0 0 1	

3698. $C_{16}H_{25}NO_2$
Nonyl *p*-aminobenzoate
Nonyl 4-aminobenzoate
RN: 37139-21-2 **MP** (°C)**:**
MW: 263.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-06	2.687E-04	37	F006	1 1 2 2 2	

3699. $C_{16}H_{25}NO_3$
4-Propoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 15788-85-9 **MP** (°C)**:**
MW: 279.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.257E-01	ns	M066	0 0 0 0 1	

3700. $C_{16}H_{26}$
2-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-08	5.678E-06	25	S377	0 0 0 0 0	

3701. $C_{16}H_{26}$
3-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	8.299E-06	25	S377	0 0 0 0 0	

3702. $C_{16}H_{26}$
4-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-08	7.862E-06	25	S377	0 0 0 0 0	

3703. $C_{16}H_{26}$
5-Phenyldecane
RN: **MP** (°C)**:**
MW: 218.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-08	7.643E-06	25	S377	0 0 0 0 0	

3704. $C_{16}H_{26}N_2O_2$
4-Propylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-54-3 **MP** (°C)**:**
MW: 278.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	2.867E-01	ns	M066	0 0 0 0 2	

3705. $C_{16}H_{26}O_2$
4-Octylphenol monoethoxylate
RN: 51437-89-9 **MP** (°C)**:**
MW: 250.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.195E-05	8.000E-03	20.5	A335	0 0 0 0 0	
3.200E-05	8.012E-03	20.5	A335	0 0 0 0 0	

3706. $C_{16}H_{26}O_5$
Artemether
RN: 71963-77-4 **MP** (°C)**:**
MW: 298.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		ns	K444	0 0 0 0 0	

3707. $C_{16}H_{26}O_6$

Triethylene glycol dibutyrate

RN: 26962-26-5 **MP** (°C)**:**
MW: 314.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.524E-02	7.937E+00	ns	F014	0 0 0 0 2	

3708. $C_{16}H_{28}N_3O_2$

Dioxyethylaminoazobenzene

RN: **MP** (°C)**:**
MW: 294.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.945E-04	8.670E-02	0	K036	1 0 0 0 2	
4.212E-04	1.240E-01	25	K036	1 0 0 0 2	
2.819E-03	8.300E-01	90	K036	1 0 0 0 2	

3709. $C_{16}H_{32}O_2$

Palmitic acid

Hexadecanoic acid

RN: 57-10-3 **MP** (°C)**:** 56
MW: 256.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.794E-05	4.600E-03	0	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20.0	R001	1 1 1 1 1	
3.200E-06	8.206E-04	25	J001	1 0 2 1 1	
1.200E-07	3.077E-05	25	R002	0 0 0 0 0	intrinsic
2.680E-06	6.872E-04	25	R002	0 0 0 0 0	
3.237E-05	8.300E-03	30	B136	1 0 2 1 1	
3.237E-05	8.300E-03	30.0	R001	1 1 1 1 1	
3.900E-05	1.000E-02	45	B136	1 0 2 1 1	
3.900E-05	1.000E-02	45.0	R001	1 1 1 1 1	
4.000E-06	1.026E-03	50	J001	1 0 2 1 1	
4.680E-05	1.200E-02	60	B136	1 0 2 1 1	
4.680E-05	1.200E-02	60.0	R001	1 1 1 1 1	
1.794E-05	4.600E-03	.0	R001	1 1 1 1 1	

3710. $C_{16}H_{34}$
2,2,4,4,6,8,8-Heptamethylnonane
RN: 4390-04-9 **MP** (°C)**:**
MW: 226.45 **BP** (°C)**:** 240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.369E-09	3.100E-07	25	T423	0 0 0 0 0	

3711. $C_{16}H_{34}$
3-Methylpentadecane
RN: 2882-96-4 **MP** (°C)**:** –22
MW: 226.45 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.328E-10	9.800E-08	23	C332	0 0 0 0 0	

3712. $C_{16}H_{34}$
Hexadecane
n-Hexadecane
Cetane
RN: 544-76-3 **MP** (°C)**:** 18.17
MW: 226.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-08	6.290E-06	25	F004	0 0 0 0 0	

3713. $C_{16}H_{34}$
2-Methylpentadecane
RN: 1560-93-6 **MP** (°C)**:** –7
MW: 226.45 **BP** (°C)**:** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.681E-10	1.060E-07	23	C332	0 0 0 0 0	

3714. $C_{16}H_{34}O$
Hexadecanol
Cetyl alcohol
RN: 36653-82-4 **MP** (°C)**:** 49
MW: 242.45 **BP** (°C)**:** 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.699E-07	4.120E-05	22.5	G301	0 0 0 0 0	
1.700E-07	4.122E-05	25	R002	0 0 0 0 0	
3.300E-08	8.001E-06	34	K011	1 2 1 1 2	

(*continued*)

3714. $C_{16}H_{34}O$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.393E-08	1.550E-05	43	H030	2 2 2 2 2	
6.393E-08	1.550E-05	43	H103	1 2 2 2 2	
1.270E-07	3.079E-05	55	K011	1 2 1 1 2	
1.675E-07	4.060E-05	61	H030	2 2 2 2 2	
1.675E-07	4.060E-05	61	H103	1 2 2 2 2	

3715. $C_{16}H_{35}O_3P$

Dibutyl isooctyl phosphonate

RN: 108979-58-4 **MP** (°C)**:**
MW: 306.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3716. $C_{16}H_{35}O_4P$

Dibutyl octyl phosphate

RN: 25786-28-1 **MP** (°C)**:**
MW: 322.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.10E-04	<1.00E-01	25	B070	1 2 0 1 0	

3717. $C_{17}H_{11}NO_3$

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-phenyl-

RN: 74103-09-6 **MP** (°C)**:**
MW: 277.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-07	3.300E-05	25	P089	0 0 0 0 0	
1.388E-07	3.850E-05	37	P089	0 0 0 0 0	
1.677E-07	4.650E-05	51	P089	0 0 0 0 0	

3718. $C_{17}H_{12}$

1,2-Benzofluorene
Benzo[a]fluorene
11H-Benzo[a]fluorene

RN: 238-84-6 **MP** (°C)**:** 187
MW: 216.29 **BP** (°C)**:** 407

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-07	4.500E-05	25	M064	1 1 2 2 1	
2.100E-07	4.542E-05	25	M342	1 0 1 1 1	
2.081E-07	4.500E-05	ns	M344	0 0 0 0 2	

3719. $C_{17}H_{12}$

2,3-Benzofluorene
Benzo[b]fluorene
11H-Benzo[b]fluorene
RN: 243-17-4 **MP** (°C)**:** 209
MW: 216.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E-08	4.000E-06	25	B319	2 0 1 2 0	
9.247E-09	2.000E-06	25	M064	1 1 2 2 1	
9.250E-09	2.001E-06	25	M342	1 0 1 1 2	

3720. $C_{17}H_{12}ClFN_2O$

Nuarimol
Triminol
Trimidal
Gauntlet
2-Chloro-4′-fluoro-α-(5-pyrimidinyl)benzhydryl alcohol
α-(2-Chlorophenyl)-α-(4-fluorophenyl)-5-pyrimidinemethanol
RN: 63284-71-9 **MP** (°C)**:**
MW: 314.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	2.618E-02	ns	R427	0 0 0 0 0	

3721. $C_{17}H_{12}ClFN_3O_2$

α-(4-Chlorophenyl)-α-(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
X-7801
DuP 860
RN: **MP** (°C)**:**
MW: 344.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.612E-06	1.590E-03	22	M362	1 1 2 1 1	

3722. $C_{17}H_{12}ClNO_2S$

Fentiazac
4-(*p*-Chlorophenyl)-2-phenyl-5-thiazoleacetic acid
RN: 18046-21-4 **MP** (°C)**:** 161.1
MW: 329.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-06	3.100E-03	5	F306	1 0 1 2 2	intrinsic
9.600E-05	3.166E-02	25	C314	0 0 0 0 0	
9.612E-05	3.170E-02	25	C314	0 0 0 0 0	

(*continued*)

3722. $C_{17}H_{12}ClNO_2S$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.080E-05	3.562E-03	25	F306	1 0 1 2 2	intrinsic
1.310E-05	4.320E-03	37	F306	1 0 1 2 2	intrinsic
1.072E-05	3.534E-03	ns	R427	0 0 0 0 0	

3723. $C_{17}H_{12}Cl_2N_2O$

Fenarimol
2,4′-Dichloro-α-(5-pyrimidinyl)benzhydryl alcohol
α-(2-Chlorophenyl)-α-(4-chlorophenyl)-5-pyrimidinemethanol
Tebulan
Rubigan 4AS
Rimidin

RN: 60168-88-9 **MP** (°C)**:** 118
MW: 331.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.136E-05	1.370E-02	25	M161	1 0 0 0 2	pH 7

3724. $C_{17}H_{12}Cl_2N_4$

Triazolam
8-Chloro-6-(*o*-chlorophenyl)-1-methyl-4H-*s*-triazolo[4,3-a][1,4]benzodiazepine
Apo-Triazo
Gen-Triazolam
Halcion
Novo-Triolam

RN: 28911-01-5 **MP** (°C)**:**
MW: 343.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.741E-05	3.000E-02	amb	L434	0 0 0 0 0	

3725. $C_{17}H_{12}Cl_{10}O_3$

Kelevan
Allied GC 9160
Despirol

RN: 4234-79-1 **MP** (°C)**:** 91
MW: 618.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.888E-06	5.500E-03	20	M164	1 0 0 0 1	

3726. $C_{17}H_{12}I_2O_3$
Benziodarone
Algocor
Amplivix
Dilafurane
RN: 68-90-6 **MP** (°C)**:**
MW: 518.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-05	5.881E-03	20	H301	0 0 0 0 0	

3727. $C_{17}H_{12}O_6$
Aflatoxin B1
AFB1
RN: 1162-65-8 **MP** (°C)**:** 268
MW: 312.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.803E-05	1.500E-02	ns	I306	0 0 0 0 0	

3728. $C_{17}H_{12}O_7$
Aflatoxin G1
RN: 1165-39-5 **MP** (°C)**:** 244
MW: 328.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.569E-05	1.500E-02	ns	I306	0 0 0 0 0	

3729. $C_{17}H_{13}ClN_4$
Alprazolam
8-Chloro-1-methyl-6-phenyl-4H-*s*-triazolo[4,3-a][1,4]benzodiazepine
Apo-Alpraz
Kalma
Novo-Alprazol
Nu-Alpraz
RN: 28981-97-7 **MP** (°C)**:**
MW: 308.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.267E-04	7.000E-02	amb	L434	0 0 0 0 0	
3.239E-04	1.000E-01	amb	L445	0 0 0 0 0	intrinsic

3730. $C_{17}H_{13}ClO_3$
Itanoxone
2′-Chloro-α-methylene-γ-oxo[1,1′-biphenyl]-4-butanoic acid
F 1379
RN: 58182-63-1 **MP** (°C)**:** 212
MW: 300.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.318E-04	1.900E-01	20	C112	2 0 1 1 2	

3731. $C_{17}H_{13}Cl_2N_3O_2$
α-(2,4-Difluorophenyl)-α-(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
A-9991
DuP 991
RN: **MP** (°C)**:**
MW: 362.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-05	7.000E-03	22	M362	1 1 2 1 1	

3732. $C_{17}H_{14}F_3N_3O_2S$
Celecoxib
4-[5-(4-Methylphenyl)-3-(trifluoromethyl)
Celebrex
SC-58635
YM-177
RN: 169590-42-5 **MP** (°C)**:**
MW: 381.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-05	7.000E-03	25	S415	0 0 0 0 0	
7.866E-06	3.000E-03	37	Y412	0 0 0 0 0	

3733. $C_{17}H_{14}N_2O$
1-*o*-Tolylazo-2-naphthol
Orange OT
Oil orange SS
1-(*o*-Tolylazo)-2-naphthol
RN: 2646-17-5 **MP** (°C)**:** 131
MW: 262.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-07	2.000E-04	30	R430	0 0 0 0 0	
1.000E-07	2.623E-05	rt	M163	0 0 0 0 1	

3734. $C_{17}H_{14}O_4S$

Rofecoxib
4-(4-Methylsulfonylphenyl)-3-phenyl-5H-furan-2-one
RN: 162011-90-7 **MP** (°C)**:**
MW: 314.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.605E-05	8.190E-03	24.99	D414	0 0 0 0 0	
2.863E-05	9.000E-03	25	S415	0 0 0 0 0	
2.977E-05	9.360E-03	29.99	D414	0 0 0 0 0	
3.556E-05	1.118E-02	34.99	D414	0 0 0 0 0	
2.545E-06	8.000E-04	37	Y421	0 0 0 0 0	

3735. $C_{17}H_{14}O_6$

Aflatoxin B2
RN: 7220-81-7 **MP** (°C)**:** 286
MW: 314.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-05	1.500E-02	ns	I306	0 0 0 0 0	

3736. $C_{17}H_{14}O_7$

Aflatoxin G2
RN: 7241-98-7 **MP** (°C)**:** 237
MW: 330.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.500E-02	ns	I306	0 0 0 0 0	

3737. $C_{17}H_{15}NO_3$

Cinnamyl acetaminophen
Cinnamic acid, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, cinnamate (ester)
RN: 20682-28-4 **MP** (°C)**:** 200–201
MW: 281.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.977E-06	1.400E-03	37	D029	0 0 0 0 0	

3738. $C_{17}H_{15}NO_5$

Benzoic acid, 2-(acetyloxy)-, 4-(acetylamino)phenyl ester

RN: 5003-48-5 **MP** (°C)**:** 174.5
MW: 313.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.383E-05	2.000E-02	21	N335	0 0 0 0 0	

3739. $C_{17}H_{16}Br_2O_3$

Bromopropylate
1-Methylethyl-4-bromo-α-(4-bromophenyl)-α-hydroxybenzeneacetate
Neoron
GS-19851
Phenisobromolate

RN: 18181-80-1 **MP** (°C)**:** 77
MW: 428.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.17E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.168E-05	5.000E-03	20	M161	1 0 0 0 0	

3740. $C_{17}H_{16}ClFN_2O_2$

Progabide
Butanamide, 4-[[(4-chlorophenyl)(5-fluoro-2-hydroxyphenyl)methylene]amino]-
Gabrene
SL 76-002

RN: 62666-20-0 **MP** (°C)**:**
MW: 334.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-04	3.716E-02	37	F309	1 0 2 2 2	
1.110E-04	3.716E-02	37	F318	2 2 0 0 2	

3741. $C_{17}H_{16}Cl_2O_3$

Chloropropylate
1-Methylethyl-4-chloro-α-(4-chlorophenyl)-α-hydroxybenzenacetate
Chlormite
Acaralate
G-24163
Rospin

RN: 5836-10-2 **MP** (°C)**:** 74
MW: 339.22 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.422E-06	1.500E-03	20	F311	1 2 2 2 1	
2.948E-05	1.000E-02	rt	M161	0 0 0 0 1	

3742. $C_{17}H_{16}N_2O_2S$
1-Sulfamethylnaphthalene
RN: **MP** (°C)**:**
MW: 312.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-05	1.000E-02	20	F073	1 2 2 2 1	

3743. $C_{17}H_{16}N_2O_3$
C.I. Disperse blue 3
1-[(2-Hydroxyethyl)amino]-4-(methylamino)-9,10-anthracenedione
C.I. 61505
RN: 2475-46-9 **MP** (°C)**:** 187
MW: 296.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.556E-05	25	B333	0 0 0 0 0	

3744. $C_{17}H_{16}N_2O_3S$
4-Sulfahydroxymethylnaphthalene
RN: **MP** (°C)**:**
MW: 328.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-04	5.500E-02	20	F073	1 2 2 2 1	

3745. $C_{17}H_{16}N_2O_4$
p-(*p*-Acetamidobenzamido)phenyl acetate
RN: 74973-19-6 **MP** (°C)**:**
MW: 312.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-05	1.218E-02	25	A066	1 0 1 1 1	

3746. $C_{17}H_{16}N_2O_4S$
1-Benzenesulfonyl-5-ethyl-5-phenyl-hydantoin
5-Ethyl-5phenyl-1(phenylsulfonyl)-2,4-imidazolidinedione
RN: 21413-25-2 **MP** (°C)**:**
MW: 344.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.782E-04	3.369E-01	37	F183	1 0 1 1 1	intrinsic

3747. $C_{17}H_{16}N_2O_5$

p-4-Acetaminophenyl acetaminophen
Acetamide, *N,N′*-[carbonylbis(oxy-4,1-phenylene)]*bis*-
Acetanilide, 4′-hydroxy-, carbonate (2:1) (ester)
RN: 19872-72-1 **MP** (°C)**:** 219.5–220
MW: 328.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-04	6.000E-02	37	D029	0 0 0 0 0	

3748. $C_{17}H_{17}ClO_6$

Griseofulvin
(2*S-trans*)-7-Chloro-2′,4,6-trimethoxy-6′-methylspiro[benzofuran-2(3H),1′-[2]cyclohexene]-3,4′-dione
Fulvicin
Grisactin
Grifulvin
Griseostatin
RN: 126-07-8 **MP** (°C)**:** 220.0
MW: 352.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-05	6.456E-03	15	E010	2 2 2 2 2	
2.466E-05	8.700E-03	20	N322	0 0 0 0 0	
3.260E-05	1.150E-02	21	E316	0 0 0 0 0	
3.175E-04	1.120E-01	21	M044	2 0 2 2 2	*sic*
4.025E-04	1.420E-01	21	M044	2 0 2 2 2	microsize, *sic*
2.126E-05	7.500E-03	22	C040	2 0 2 2 0	EFG
2.076E-05	7.325E-03	22	M382	2 1 1 1 1	average of 2
1.474E-05	5.200E-03	22.5	B422	2 0 2 2 2	
2.523E-05	8.900E-03	23	B362	0 0 0 0 0	
2.268E-05	8.000E-03	25	C037	2 1 2 2 2	
2.450E-05	8.643E-03	25	E010	2 2 2 2 2	
3.685E-05	1.300E-02	25	H015	1 0 0 0 1	
2.835E-05	1.000E-02	25	L033	1 0 2 1 1	
2.268E-05	8.000E-03	25	M457	0 0 0 0 0	
2.750E-05	9.700E-03	25	P096	0 0 0 0 0	
2.551E-05	9.000E-03	27	B043	1 0 1 2 0	EFG
2.835E-05	1.000E-02	30	M045	2 0 0 0 0	
4.000E-05	1.411E-02	30	O321	0 0 0 0 0	
4.252E-05	1.500E-02	30	O321	0 0 0 0 0	
3.510E-05	1.238E-02	35	E010	2 2 2 2 2	
3.969E-05	1.400E-02	37	B039	2 1 1 1 0	EFG
4.252E-05	1.500E-02	37	B043	1 0 1 2 0	EFG
3.969E-05	1.400E-02	37	B045	1 0 1 1 1	
4.054E-05	1.430E-02	37	F033	2 0 2 0 2	
3.968E-05	1.400E-02	37	G011	1 0 1 1 0	EFG
4.252E-05	1.500E-02	37	K018	1 0 0 0 1	
5.669E-05	2.000E-02	45	B043	1 0 1 2 0	EFG

(*continued*)

3748. $C_{17}H_{17}ClO_6$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.140E-05	2.166E-02	45	E010	2 2 2 2 2	
3.798E-05	1.340E-02	ns	D340	0 0 0 0 0	
2.835E-04	1.000E-01	ns	K444	0 0 0 0 0	
2.466E-05	8.700E-03	ns	N323	0 0 0 0 0	

3749. $C_{17}H_{17}Cl_2N$

Sertraline

(1*S*-*cis*)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-*N*-methyl-1-naphthalenamine

RN: 79617-96-2 **MP** (°C)**:**

MW: 306.24 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.27E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3750. $C_{17}H_{17}NO_2$

Apomorphine

Apomorphin

RN: 58-00-4 **MP** (°C)**:**

MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.069E-01	15	K059	2 2 2 0 0	
7.481E-02	2.000E+01	25	P312	0 0 0 0 0	

3751. $C_{17}H_{17}NO_5$

N-Benzyloxycarbonyl-L-tyrosine

Carbobenzoxytyrosine

RN: 1164-16-5 **MP** (°C)**:**

MW: 315.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.852E-03	1.530E+00	25.1	N026	0 0 0 0 0	

3752. $C_{17}H_{17}N_5O_5$

9-[5′-(*O*-Benzoyl)-β-D-arabinofuranosyl]adenine ester

RN: 42782-57-0 **MP** (°C)**:** 223.0

MW: 371.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E-04	8.000E-02	ns	B134	0 1 1 1 0	

3753. $C_{17}H_{18}ClNO_6$

Griseofulvin-4′-oxime

Spiro[benzofuran-2(3H),1′-[2]cyclohexene]-3,4′-dione, 7-chloro-2′,4,6-trimethoxy-6′-methyl-, 4′-oxime

RN: 13215-54-8 **MP** (°C)**:**
MW: 367.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.589E-04	1.320E-01	37	F033	2 0 2 0 2	

3754. $C_{17}H_{18}ClN_5O_6$

Dis. A. 8

Ethanol, 2,2′-[[4-[(2-chloro-4,6-dinitrophenyl)azo]-3-methylphenyl]imino]*bis*-

RN: 65125-87-3 **MP** (°C)**:**
MW: 423.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.119E-04	25	B333	0 0 0 0 0	

3755. $C_{17}H_{18}Cl_2N_4O_4$

Dis. A. 10

Ethanol, 2,2′-[4-(2,6-dichloro-4-nitrophenylazo)-*m*-tolylimino]di-

RN: 58528-60-2 **MP** (°C)**:**
MW: 413.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.546E-04	25	B333	0 0 0 0 0	

3756. $C_{17}H_{18}FN_3O_3$

Ciprofloxacin

1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic

Baycip

Velmonit

RN: 85721-33-1 **MP** (°C)**:**
MW: 331.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.117E-04	3.700E-02	6	Y421	0 0 0 0 0	
1.630E-04	5.400E-02	22.5	B422	2 0 2 2 2	
2.595E-04	8.600E-02	25	Y421	0 0 0 0 0	
4.225E-04	1.400E-01	30	Y421	0 0 0 0 0	
5.131E-04	1.700E-01	40	Y421	0 0 0 0 0	
3.730E+00	1.236E+03	c	B443	0 0 0 0 0	

3757. $C_{17}H_{18}N_2O_6$
Nifedipine
3,5-Pyridinedicarboxylicacid
RN: 21829-25-4 **MP** (°C)**:** 172–174
MW: 346.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-05	5.800E-03	25	B387	0 0 0 0 0	
2.887E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.738E-05	6.019E-03	ns	R427	0 0 0 0 0	

3758. $C_{17}H_{18}N_4O_3S$
4-Sulfanilamido-1-phenyl-2,3-dimethyl-5-pyrazolone
RN: 71119-16-9 **MP** (°C)**:**
MW: 358.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.352E-04	1.560E-01	37	R045	1 2 1 1 2	

3759. $C_{17}H_{19}ClN_2S$
4-Chloropromazine
4-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 13094-24-1 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-05	3.508E-03	ns	G023	0 0 1 1 1	

3760. $C_{17}H_{19}ClN_2S$
3-Chloropromazine
3-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 484-19-5 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.189E-03	ns	G023	0 0 1 1 1	

3761. $C_{17}H_{19}ClN_2S$
1-Chloropromazine
1-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 13100-13-5 **MP** (°C)**:**
MW: 318.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	3.826E-03	0	G023	0 0 0 0 1	

3762. $C_{17}H_{19}ClN_4O_4$

C.I. Disperse red 5

Ethanol, 2,2′-[[4-[(2-chloro-4-nitrophenyl)azo]-3-methylphenyl]imino]*bis*-

RN: 3769-57-1 **MP** (°C)**:** 192

MW: 378.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.440E-04	25	B333	0 0 0 0 0	

3763. $C_{17}H_{19}ClO_6$

Griseofulvin-4′-ol

Spiro[benzofuran-2(3H),1′-[2]cyclohexen]-3-one, 7-chloro-4′-hydroxy-2′,4,6-trimethoxy-6′-methyl-

RN: 13215-53-7 **MP** (°C)**:**

MW: 354.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E-04	2.529E-01	37	F033	2 0 2 0 2	average of 2

3764. $C_{17}H_{19}NO_3$

Piperine

Piperidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]-, (E,E)-

N-[(E,E)-Piperoyl]piperidine

RN: 94-62-2 **MP** (°C)**:** 130.0

MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	3.995E-02	15	K059	2 2 2 0 1	
1.402E-04	4.000E-02	18	F300	1 0 0 0 0	
3.504E-04	9.999E-02	rt	D021	0 0 1 1 0	

3765. $C_{17}H_{19}NO_3$

1-Methyl-1-nitro-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane

RN: 53982-07-3 **MP** (°C)**:**

MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.060E-06	2.300E-03	rt	C122	0 0 0 0 0	

3766. $C_{17}H_{19}NO_3$

Hydromorphone
Dilaudid
PMS-Hydromorphone
Dihydromorphinone

RN: 466-99-9 **MP** (°C)**:**
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.767E-03	1.931E+00	25	R338	0 0 0 0 0	

3767. $C_{17}H_{19}NO_3$

Morphine
Morphin
7,8-Didehydro-4,5-epoxy-17-methylmorphinan-3,6-diol

RN: 57-27-2 **MP** (°C)**:** 254dec
MW: 285.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.427E-01	15	K059	2 2 2 0 0	
5.222E-04	1.490E-01	20	B061	1 0 1 1 2	
5.257E-04	1.500E-01	20	F300	1 0 0 0 0	
1.209E-03	3.450E-01	25	R338	0 0 0 0 0	
7.200E-04	2.054E-01	30	L068	1 0 0 1 0	EFG
1.000E-03	2.853E-01	30	L069	1 0 1 1 0	EFG
8.761E-04	2.500E-01	35	R418	0 0 0 0 0	Intrinsic
1.051E-03	2.999E-01	rt	D021	0 0 1 1 0	

3768. $C_{17}H_{19}NO_3.H_2O$

Morphine (monohydrate)
Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl-(5α,6α)-, monohydrate

RN: 6009-81-0 **MP** (°C)**:** 254dec
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.328E-04	2.830E-01	c	D004	0 0 0 0 0	
3.064E-03	9.294E-01	h	D004	0 0 0 0 0	

3769. $C_{17}H_{19}NO_4$

1-Methyl-1-nitro-2,2-bis(*p*-methoxylphenyl)ethane

RN: 34197-26-7 **MP** (°C)**:**
MW: 301.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.854E-05	8.600E-03	rt	C122	0 0 0 0 0	

3770. $C_{17}H_{19}N_3$
Antazoline
Albalon-A
RN: 91-75-8 **MP** (°C)**:** 120
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	6.634E-01	30	L068	1 0 0 1 0	EFG
1.900E-02	5.042E+00	37.5	L034	2 2 0 1 2	pH 7.4

3771. $C_{17}H_{19}N_5O_6$
Dis. A. 1
Ethanol, 2,2′-[4-(2,4-dinitrophenylazo)-*m*-tolylimino]di-
Disperse violet 4K
Terasil violet P 4RT
RN: 41541-13-3 **MP** (°C)**:** 190
MW: 389.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-07	2.726E-04	25	B333	0 0 0 0 0	

3772. $C_{17}H_{20}ClN_5O_2$
1H-Purine-2,6-dione, 8-(2-amino-4-chlorophenyl)-3,7-dihydro-1,3-dipropyl-
1,3-Dipropyl-8-(2-amino-4-chlorophenyl)xanthine
PACPX
RN: 85872-51-1 **MP** (°C)**:**
MW: 361.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.76E-07	<1.00E-04	ns	H316	0 0 0 0 0	pH 7.4
1.105E-06	4.000E-04	ns	H316	0 0 0 0 0	0.1N HCL

3773. $C_{17}H_{20}N_2O$
Michler′s ketone
Tetramethyldiaminobenzophenone
bis[4-(Dimethylamino)phenyl]-methanone
p,p′-bis(*N,N*-Dimethylamino)benzophenone
4,4[-bis(Dimethylamino)benzophenone
RN: 90-94-8 **MP** (°C)**:** 172.0
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	3.998E-01	rt	D021	0 0 1 1 0	

3774. $C_{17}H_{20}N_2O_2$

Tropicamide

RN: 1508-75-4 **MP** (°C)**:**
MW: 284.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.032E-04	2.000E-01	25	C414	1 0 1 1 0	EFG

3775. $C_{17}H_{20}N_2S$

Promethazine
10-(2-Dimethylaminopropyl)phenothiazine
10-(2-Dimethylamino-2-methylethyl)phenothiazine
Fenergan
Protazine
Thiergan

RN: 60-87-7 **MP** (°C)**:** 60
MW: 284.43 **BP** (°C)**:** 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-06	3.839E-04	22.5	B440	0 0 0 0 0	
5.500E-05	1.564E-02	24	G023	2 0 1 1 1	
4.390E+00	1.249E+03	c	B443	0 0 0 0 0	

3776. $C_{17}H_{20}N_2S$

Promazine
Primazine
Sparine
Prozine

RN: 58-40-2 **MP** (°C)**:** 32
MW: 284.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.422E-02	24	G023	2 0 1 1 1	
5.000E-05	1.422E-02	ns	G023	0 0 0 0 1	

3777. $C_{17}H_{20}N_4O_4$

C.I. Disperse red 17
Ethanol, 2,2′-[[3-methyl-4-[(4-nitrophenyl)azo]phenyl]imino]*bis*-

RN: 3179-89-3 **MP** (°C)**:** 160
MW: 344.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	6.199E-04	25	B333	0 0 0 0 0	

3778. $C_{17}H_{20}N_4O_5$

Dis. A. 13
4-Nitro-2-methoxy-4′-di(β-hydroxyethyl)-aminoazobenzene
Ethanol, 2,2′-[[4-[(2-methoxy-4-nitrophenyl)azo]phenyl]imino]bis
Ethanol, 2,2′-[*p*-(2-methoxy-4-nitrophenylazo)phenylimino]di-
RN: 41541-14-4 **MP** (°C)**:**
MW: 360.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.207E-03	25	B333	0 0 0 0 0	
6.826E-04	2.460E-01	100	P313	0 0 0 0 0	

3779. $C_{17}H_{20}N_4O_5S$

Benzenesulfonic acid, 4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-
RN: 89073-57-4 **MP** (°C)**:**
MW: 392.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	1.300E+00	ns	H316	0 0 0 0 0	0.1N HCL
>6.12E-02	>2.40E+01	ns	H316	0 0 0 0 0	pH 7.4

3780. $C_{17}H_{20}N_4O_6$

Riboflavine
Riboflavin
Robiflavine
7,8-Dimethyl-10-ribitylisoalloxazine
Zinvit-G
E-101
RN: 83-88-5 **MP** (°C)**:** 290
MW: 376.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.657E-04	9.999E-02	20	A022	1 0 0 0 0	
2.250E-04	8.468E-02	25	A079	1 0 1 1 2	
2.657E-04	9.999E-02	25	D041	1 0 0 0 0	
1.754E-04	6.600E-02	25	D315	0 0 0 0 0	
2.192E-04	8.250E-02	30	C409	2 0 1 2 2	
3.959E-04	1.490E-01	37	E018	1 0 2 1 2	
2.089E-04	7.864E-02	ns	R427	0 0 0 0 0	

3781. $C_{17}H_{20}O_6$

Mycophenolic acid
6-(1,3-Dihydro-7-hydroxy-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic acid
RN: 24280-93-1 **MP** (°C)**:**
MW: 320.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.058E-05	1.300E-02	25	L333	1 1 1 1 0	

3782. $C_{17}H_{21}NO_2$

Napropamide
N,N-Diethyl-2-(1-naphthyloxy)propanamide
Devrinol 50W
Devrinol
Devrinol 10G
Devrinol 2E
RN: 15299-99-7 **MP** (°C)**:** 75.1
MW: 271.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	7.300E-02	20	M161	1 0 0 0 1	

3783. $C_{17}H_{21}NO_3$

Etodolac
(+/-)-1,8-Diethyl-1,3,4,9-tetrahydropyrano-(3,4-b)indole-1-acetic acid
Lodine
RN: 41340-25-4 **MP** (°C)**:**
MW: 287.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E-04	4.000E-02	37	Y421	0 0 0 0 0	

3784. $C_{17}H_{21}NO_4$

Scopolamine
Scopolamin
Hyoscine
Murocoll
Plexonal
Transderm-SCOP
RN: 51-34-3 **MP** (°C)**:** 59
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E-01	9.500E+01	15	F300	1 0 0 0 1	
3.296E-01	1.000E+02	ns	C109	0 0 0 0 1	

3785. $C_{17}H_{21}NO_4$
Cocaine
L-Cocaine
L-Cocain
RN: 50-36-2 **MP** (°C)**:** 98
MW: 303.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	1.213E+00	15	K059	2 2 2 0 0	
5.934E-03	1.800E+00	22	F300	1 0 0 0 1	
5.485E-03	1.664E+00	25	D004	0 0 0 0 0	
5.266E-03	1.597E+00	25	D041	1 0 0 0 1	
1.248E-02	3.786E+00	80	D041	1 0 0 0 1	

3786. $C_{17}H_{21}N_3O_2$
Dis. A. 2
Ethanol, 2,2′-[[3-methyl-4-(phenylazo)phenyl]imino]*bis*-
4-[bis(2-Hydroxyethyl)amino]-2-methylazobenzene
RN: 3771-38-8 **MP** (°C)**:** 111
MW: 299.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-05	2.275E-02	25	B333	0 0 0 0 0	

3787. $C_{17}H_{21}N_5O_2$
1H-Purine-2,6-dione, 8-(2-aminophenyl)-3,7-dihydro-1,3-dipropyl-
RN: 96445-34-0 **MP** (°C)**:** 276dec
MW: 327.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.05E-06	<1.00E-03	ns	H316	0 0 0 0 0	pH 7.4
1.222E-05	4.000E-03	ns	H316	0 0 0 0 0	0.1N HCL

3788. $C_{17}H_{21}N_5O_{10}$
9-(1,3-Dihemisuccinate-2-propoxymethyl)guanine
RN: 88110-76-3 **MP** (°C)**:** 167
MW: 455.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	4.730E+01	25	B360	0 0 0 0 0	

3789. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*RS**)]-

RN: 60166-94-1 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3790. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*RS**)]-

RN: 77942-93-9 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-01	1.150E+02	25	P091	0 0 0 0 0	

3791. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N′*-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-

RN: 77868-45-2 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3792. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*S*-(*S**,*S**)]-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3793. $C_{17}H_{22}I_3N_3O_8$

DL-Iopamidol

1,3-Benzenedicarboxamide, *N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-

L-Iopamidol

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*S**,*S**)]-

RN: 60166-93-0 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-01	4.737E+02	20	F178	1 0 0 0 1	EFG
1.580E-01	1.228E+02	20	F178	1 0 0 0 1	EFG
6.096E-01	4.737E+02	25	P091	0 0 0 0 0	
1.580E-01	1.228E+02	25	P091	0 0 0 0 0	
5.798E-01	4.505E+02	40	F178	1 0 0 0 1	EFG
1.963E-01	1.525E+02	40	F178	1 0 0 0 1	EFG
5.679E-01	4.413E+02	60	F178	1 0 0 0 1	EFG
3.120E-01	2.424E+02	60	F178	1 0 0 0 1	EFG
6.235E-01	4.845E+02	80	F178	1 0 0 0 1	EFG
5.209E-01	4.048E+02	80	F178	1 0 0 0 1	EFG
6.911E-01	5.370E+02	100	F178	1 0 0 0 1	EFG
7.098E-01	5.516E+02	100	F178	1 0 0 0 1	EFG

3794. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*S**)]-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3795. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*RS*)-

RN: 60208-45-9 **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-01	1.379E+02	25	P091	0 0 0 0 0	

3796. $C_{17}H_{22}I_3N_3O_8$

1,3-Benzenedicarboxamide, *N,N′*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(*RS*,*S*)-

RN: **MP** (°C)**:**
MW: 777.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3797. $C_{17}H_{22}I_3N_3O_9$

1,3-Benzenedicarboxamide, 5-[(2,3-dihydroxy-1-oxopropyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 69698-47-1 **MP** (°C)**:**
MW: 793.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.573E-02	5.213E+01	25	P091	0 0 0 0 0	

3798. $C_{17}H_{22}I_3N_3O_9$

1,3-Benzenedicarboxamide, 5-[(2,3-dihydroxy-1-oxobutyl)amino]-*N,N′*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 129968-26-9 **MP** (°C)**:**
MW: 793.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.430E-02	4.306E+01	25	P091	0 0 0 0 0	

3799. $C_{17}H_{22}N_4O_3S$

2-(*N*4-Acetylsulfanilylamino)-4-*n*-amylpyrimidine

RN: **MP** (°C)**:**
MW: 362.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.214E-05	4.400E-03	37	R076	1 2 0 0 1	

3800. $C_{17}H_{22}N_4O_7.0.75H_2O$

2′-(2-Methyl-3-one-pentanyl)-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-50-4 **MP** (°C)**:** 55–60
MW: 407.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.770E-02	3.577E+01	37	C348	0 0 0 0 0	pH 7.00

3801. $C_{17}H_{23}NO$
N,N-Octamethylenecinnamamide
Octahydro-1-(1-oxo-3-phenyl-2-propenyl)1H-azonine
RN: 59832-07-4 **MP** (°C)**:**
MW: 257.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	6.332E-02	ns	H350	0 0 0 0 0	

3802. $C_{17}H_{23}NO$
N-Cyclooctylcinnamamide
2-Propenamide, *N*-cyclooctyl-3-phenyl-
RN: 59832-00-7 **MP** (°C)**:**
MW: 257.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.660E-06	6.846E-04	ns	H350	0 0 0 0 0	

3803. $C_{17}H_{23}NO_3$
Hyoscyamine
Hyoscyamin
Benzeneacetic acid, α-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, [3(*S*)-*endo*]-
Daturine
Duboisine
L-Hyoscyamine
RN: 101-31-5 **MP** (°C)**:** 108.5
MW: 289.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.244E-02	3.600E+00	20	F300	1 0 0 0 2	
1.225E-02	3.546E+00	c	D004	0 0 0 0 0	

3804. $C_{17}H_{23}NO_3$
Atropine
Atropin
8-Methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropionate
Neo-diophen
Minims
RN: 51-55-8 **MP** (°C)**:** 115
MW: 289.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.592E+00	15	K059	2 2 2 0 1	
5.529E-03	1.600E+00	18	F300	1 0 0 0 1	

(*continued*)

3804. $C_{17}H_{23}NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E-03	1.996E+00	20	D041	1 0 0 0 0	
1.032E-02	2.987E+00	20	K052	1 1 1 1 2	
1.610E+00	4.659E+02	25	B443	0 0 0 0 0	
1.148E-02	3.322E+00	25	D004	0 0 0 0 0	
7.586E-03	2.195E+00	rt	D021	0 0 1 1 1	

3805. $C_{17}H_{23}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-[bis(1-methylethyl)amino]-2-oxoethyl ester

RN: 116482-76-9 **MP** (°C)**:** 108.9
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-04	1.800E-01	21	N335	0 0 0 0 0	

3806. $C_{17}H_{23}NO_5$

Benzoic acid, 2-(acetyloxy)-, 2-(dipropylamino)-2-oxoethyl ester

RN: 116482-75-8 **MP** (°C)**:** 50.5
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	7.200E-01	21	N335	0 0 0 0 0	

3807. $C_{17}H_{23}N_3O$

Aeo-antergan
1,2-Ethanediamine, *N*-[(4-methoxyphenyl)methyl]-*N′,N′*-dimethyl-*N*-2-pyridinyl-
Dorantamin
Anthisan
Dipane
Copsamine

RN: 91-84-9 **MP** (°C)**:**
MW: 285.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	3.425E+00	37.5	L034	2 2 0 1 2	pH 7.4

3808. $C_{17}H_{23}N_3O_2$
2-Methoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-methoxyquinoline-4-carboxamide
RN: 2716-98-5 **MP** (°C)**:**
MW: 301.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	9.042E-01	ns	B018	0 0 0 0 1	
3.000E-03	9.042E-01	ns	M066	0 0 0 0 0	

3809. $C_{17}H_{24}N_4O_5$
1,5-Dipivaloyloxymethyl allopurinol
RN: 98827-16-8 **MP** (°C)**:** 136–137
MW: 364.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.488E-05	2.000E-02	22	B322	0 0 0 0 0	
5.495E-05	2.003E-02	ns	R427	0 0 0 0 0	

3810. $C_{17}H_{24}N_4O_5$
2,5-Dipivaloyloxymethyl allopurinol
RN: 98827-17-9 **MP** (°C)**:** 145–146
MW: 364.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-04	4.500E-02	22	B322	0 0 0 0 0	

3811. $C_{17}H_{24}N_4O_6$
2′-Hexanyl-6-methoxypurine arabinoside
RN: 145913-39-9 **MP** (°C)**:**
MW: 380.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	7.190E+00	37	C348	0 0 0 0 0	pH 7.00

3812. $C_{17}H_{25}NO$
N-Octylcinnamamide
2-Propenamide, *N*-octyl-3-phenyl-
RN: 55030-48-3 **MP** (°C)**:**
MW: 259.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-06	3.606E-04	ns	H350	0 0 0 0 0	

3813. $C_{17}H_{25}NO_3$

Acetamide, 2-(benzoyloxy)-*N*,*N*-bis(2-methylpropyl)-

RN: 115193-33-4 **MP** (°C)**:** 44.5
MW: 291.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3814. $C_{17}H_{25}NO_3$

Acetamide, 2-(benzoyloxy)-*N*,*N*-acetamide, 2-(benzoyloxy)-*N*,*N*-dibutyl-

RN: 106231-57-6 **MP** (°C)**:** 25
MW: 291.39 **BP** (°C)**:** 428.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	B427	1 0 0 1 1	in 0.01M HCl
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3815. $C_{17}H_{25}NO_4$

Octyl acetaminophen
Carbonic acid, octyl ester, ester with 4′-hydroxyacetanilide
Acetanilide, 4′-hydroxy-, octyl carbonate (ester)

RN: 19872-70-9 **MP** (°C)**:** 82.5–83
MW: 307.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-05	4.400E-03	37	D029	0 0 0 0 0	

3816. $C_{17}H_{25}N_5O_6$

9-(1,3-Dibutyrate-2-propoxymethyl)guanine

RN: 88110-71-8 **MP** (°C)**:** 200
MW: 395.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-04	1.400E-01	25	B360	0 0 0 0 0	

3817. $C_{17}H_{26}ClNO_2$

Butachlor
N-(Butoxymethyl)-2-chloro-*N*-(2,6-diethylphenyl)acetamide
N-(Butoxymethyl)-2-chloro-2′,6′-diethylacetanilide
Machete
Butanex
Hiltachlor

RN: 23184-66-9 **MP** (°C)**:** <–5
MW: 311.86 **BP** (°C)**:** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.413E-05	2.000E-02	20	M161	1 0 0 0 1	
6.412E-05	2.000E-02	ns	S460	0 0 0 0 0	
7.055E-05	2.200E-02	ns	Y414	0 0 0 0 0	
7.055E-02	2.200E+01	ns	Y414	0 0 0 0 0	

3818. $C_{17}H_{26}O_3$

Decyl-*p*-hydroxybenzoate
Decyl *p*-hydroxybenzoate
n-Decyl *p*-hydroxybenzoate

RN: 69679-30-7 **MP** (°C)**:** 58
MW: 278.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	8.909E-03	15	B355	0 0 0 0 0	
3.710E-05	1.033E-02	20	B355	0 0 0 0 0	
8.800E-05	2.450E-02	25	B355	0 0 0 0 0	
1.303E-03	3.629E-01	25	D081	1 2 2 1 2	*sic*
7.943E-05	2.211E-02	25	F322	2 0 1 1 0	EFG

3819. $C_{17}H_{27}NO_2$

Terbutol
2,6-Di-*tert*-butyl-*p*-tolyl methylcarbamate

RN: 1918-11-2 **MP** (°C)**:** 185
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E-05	6.500E-03	25	B200	1 0 0 0 0	
2.523E-05	7.000E-03	ns	H042	0 0 0 0 0	

3820. $C_{17}H_{27}NO_2$
Venlafaxine
RN: 93413-69-5 **MP** (°C)**:**
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.60E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3821. $C_{17}H_{27}NO_3$
Pramoxine
Pramocaine
RN: 140-65-8 **MP** (°C)**:**
MW: 293.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-05	3.574E-03	22.5	B440	0 0 0 0 0	

3822. $C_{17}H_{27}NO_3$
Stadacain
4-Butoxybenzoic acid 2-(diethyl-amino)ethyl ester
RN: 2350-32-5 **MP** (°C)**:** 146
MW: 293.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	3.814E-02	ns	M066	0 0 0 0 1	

3823. $C_{17}H_{27}NO_4$
Nadolol
Corgard
Nadolol
RN: 42200-33-9 **MP** (°C)**:**
MW: 309.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-02	8.300E+00	25	A412	1 0 2 2 1	int

3824. $C_{17}H_{28}$
4-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-09	2.092E-06	25	S377	0 0 0 0 0	

3825. $C_{17}H_{28}$
6-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	2.557E-06	25	S377	0 0 0 0 0	

3826. $C_{17}H_{28}$
3-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-08	2.789E-06	25	S377	0 0 0 0 0	

3827. $C_{17}H_{28}$
2-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-09	1.859E-06	25	S377	0 0 0 0 0	

3828. $C_{17}H_{28}$
5-Phenylundecane
RN: **MP** (°C)**:**
MW: 232.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-08	2.324E-06	25	S377	0 0 0 0 0	

3829. $C_{17}H_{28}N_2O_2$
4-Butylaminobenzoic acid 2-(diethyl-amino)ethyl ester
RN: 3772-42-7 **MP** (°C)**:**
MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	1.199E-01	ns	M066	0 0 0 0 1	

3830. $C_{17}H_{28}N_2O_2$

Endomid

N,*N*,*N*′,*N*′-Tetraethyl-bicyclo(2.2.1)hept-5-ene-2,3-dicarboxamide

RN: 4582-18-7 **MP** (°C)**:**

MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.916E-02	1.730E+01	20	K050	1 1 1 1 2	

3831. $C_{17}H_{28}O_2$

4-Nonylphenol monoethoxylate

Ethanol, 2-(4-nonylphenoxy)-

RN: 104-35-8 **MP** (°C)**:**

MW: 264.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.048E-05	2.770E-03	2	A335	0 0 0 0 0	
1.050E-05	2.776E-03	2	A335	0 0 0 0 0	
1.063E-05	2.810E-03	10	A335	0 0 0 0 0	
1.060E-05	2.803E-03	10	A335	0 0 0 0 0	
1.074E-05	2.840E-03	14	A335	0 0 0 0 0	
1.080E-05	2.856E-03	14	A335	0 0 0 0 0	
1.140E-05	3.014E-03	20.5	A335	0 0 0 0 0	
1.142E-05	3.020E-03	20.5	A335	0 0 0 0 0	
1.280E-05	3.384E-03	25	A335	0 0 0 0 0	
1.275E-05	3.370E-03	25	A335	0 0 0 0 0	

3832. $C_{17}H_{34}O_2$

Margaric acid

Heptadecanoic acid

RN: 506-12-7 **MP** (°C)**:**

MW: 270.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-05	2.800E-03	0	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20.0	R001	1 1 1 1 1	
1.997E-05	5.400E-03	30	B136	1 0 2 1 1	
2.034E-05	5.500E-03	30.0	R001	1 1 1 1 1	
2.551E-05	6.900E-03	45	B136	1 0 2 1 1	
2.551E-05	6.900E-03	45.0	R001	1 1 1 1 1	
2.995E-05	8.100E-03	60	B136	1 0 2 1 1	
2.995E-05	8.100E-03	60.0	R001	1 1 1 1 1	
1.035E-05	2.800E-03	.0	R001	1 1 1 1 1	

3833. $C_{17}H_{36}N_2Ge$
Spirogermanium
2-[3-(Dimethylamino)propyl]-8,8-diethyl-2-aza-8-germaspiro[4.5]decane
RN: 41992-23-8 **MP** (°C)**:**
MW: 341.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-05	8.400E-03	22	M456	0 0 0 0 0	pH 12.5

3834. $C_{17}H_{36}O$
Heptadecanol
1-Heptadecanol
RN: 1454-85-9 **MP** (°C)**:** 58
MW: 256.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<=1E-7	<=2.56E-5	25	R002	0 0 0 0 0	

3835. $C_{18}H_{10}Cl_4$
2,4,4″,6-Tetrachloro-*p*-terphenyl
2,4,4″,6-Tetrachloro-1,1′:4′,1″-terphenyl
RN: 61576-97-4 **MP** (°C)**:**
MW: 368.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.606E-10	5.910E-08	4	D351	1 2 1 1 2	
4.728E-10	1.740E-07	25	D351	1 2 1 1 2	
1.106E-09	4.069E-07	40	D351	1 2 1 1 2	

3836. $C_{18}H_{10}I_6N_2O_7$
Ioglycamic acid
N,*N*′-bis(3-Carboxy-2,4,6-triiodophenyl)-diglycolamide
BE 419
RN: 2618-25-9 **MP** (°C)**:**
MW: 1127.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.773E-04	2.000E-01	ns	H055	0 0 0 0 0	

3837. $C_{18}H_{10}N_2O_2S$
Disperse brightener
2,2′-(2,5-Thiophenediyl)bisbenzoxazole
Unitex OB
Uvitex EBF
RN: 2866-43-5 **MP** (°C)**:** 219
MW: 318.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-08	9.551E-06	25	B333	0 0 0 0 0	

3838. $C_{18}H_{11}Cl_3$
2,4″,5-Trichloro-*p*-terphenyl
2,4″,5-Trichloro-1,1′:4′,1″-terphenyl
RN: 61576-93-0 **MP** (°C)**:**
MW: 333.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-10	1.010E-07	4	D351	1 2 1 1 2	
1.233E-09	4.115E-07	25	D351	1 2 1 1 2	
2.567E-09	8.564E-07	39	D351	1 2 1 1 2	

3839. $C_{18}H_{11}NO_3$
Samaron yellow
Supra light yellow GGL(IG)
RN: 1326-08-5 **MP** (°C)**:**
MW: 289.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-06	1.157E-03	98.59	M180	0 0 2 2 0	EFG
8.000E-06	2.314E-03	111.46	M180	0 0 2 2 0	EFG
1.000E-05	2.893E-03	112.94	M180	0 0 2 2 0	EFG
1.100E-05	3.182E-03	119.00	M180	0 0 2 2 0	EFG
1.300E-05	3.761E-03	125.25	M180	0 0 2 2 0	EFG
1.400E-05	4.050E-03	128.45	M180	0 0 2 2 0	EFG
2.200E-05	6.364E-03	152.37	M180	0 0 2 2 0	EFG

3840. $C_{18}H_{11}NO_3$
Disperse yellow 54
C.I. Disperse yellow 54
RN: 7576-65-0 **MP** (°C)**:**
MW: 289.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.893E-05	25	B333	0 0 0 0 0	
2.400E-07	6.943E-05	60.0	D093	1 2 1 2 0	EFG

(*continued*)

3840. $C_{18}H_{11}NO_3$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-07	1.880E-04	71.8	D093	1 2 1 2 0	EFG
1.600E-06	4.629E-04	84.1	D093	1 2 1 2 0	EFG
4.000E-06	1.157E-03	97.4	D093	1 2 1 2 0	EFG

3841. $C_{18}H_{12}$

Tetracene
Naphthacene
2,3-Benzanthracene

RN: 92-24-0 **MP** (°C)**:** 341
MW: 228.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-08	3.607E-06	20	E009	1 0 0 1 2	
6.600E-09	1.507E-06	25	K001	2 2 2 2 1	
2.497E-09	5.700E-07	25	M064	1 1 2 2 1	
2.500E-09	5.707E-07	25	M342	1 0 1 1 1	
4.380E-09	1.000E-06	27	D003	1 0 0 1 1	
2.497E-09	5.700E-07	ns	M344	0 0 0 0 2	
2.754E-09	6.288E-07	ns	R424	0 0 0 0 0	

3842. $C_{18}H_{12}$

Triphenylene
9,10-Benzphenanthrene
Isochrysene

RN: 217-59-4 **MP** (°C)**:** 199
MW: 228.30 **BP** (°C)**:** 425

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-08	2.694E-06	8	M082	1 1 1 2 2	
1.180E-08	2.694E-06	8	M151	2 1 2 2 2	
1.311E-08	2.992E-06	8.04	M183	1 2 1 1 2	
1.330E-08	3.036E-06	12.00	M082	1 1 1 2 2	
1.330E-08	3.036E-06	12.00	M151	2 1 2 2 2	
1.328E-08	3.033E-06	12.04	M183	1 2 1 1 2	
1.490E-08	3.402E-06	14.80	M082	1 1 1 2 2	
1.490E-08	3.402E-06	14.80	M151	2 1 2 2 2	
2.500E-07	5.707E-05	20	E009	1 0 0 1 1	
2.140E-08	4.886E-06	20.50	M082	1 1 1 2 2	
2.140E-08	4.886E-06	20.50	M151	2 1 2 2 2	
2.144E-08	4.894E-06	20.54	M183	1 2 1 1 2	
1.800E-07	4.109E-05	25	A325	2 1 2 2 1	
1.880E-07	4.292E-05	25	K001	1 0 2 1 2	
1.884E-07	4.300E-05	25	M064	1 1 2 2 1	
2.891E-08	6.600E-06	25.00	M151	2 1 1 2 1	
1.665E-07	3.800E-05	27	D003	1 0 0 1 1	
3.350E-08	7.648E-06	27.30	M082	1 1 1 2 2	

(*continued*)

3842. $C_{18}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.350E-08	7.648E-06	27.30	M151	2 1 2 2 2	
3.354E-08	7.657E-06	27.34	M183	1 2 1 1 2	
3.550E-08	8.105E-06	28.20	M082	1 1 1 2 2	
3.550E-08	8.105E-06	28.20	M151	2 1 2 2 2	
3.556E-08	8.117E-06	28.24	M183	1 2 1 1 2	
1.486E-08	3.393E-06	114.84	M183	1 2 1 1 2	
1.884E-07	4.300E-05	ns	M344	0 0 0 0 2	

3843. $C_{18}H_{12}$

1,2-Benzanthracene
Benzanthracene
1,2-Benzoanthracene

RN: 56-55-3 **MP** (°C)**:** 155
MW: 228.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-08	2.991E-06	6.90	M082	1 1 1 2 2	
1.310E-08	2.991E-06	6.90	M151	2 1 2 2 2	
1.311E-08	2.992E-06	6.94	M183	1 2 1 1 2	
1.660E-08	3.790E-06	10.70	M082	1 1 1 2 2	
1.660E-08	3.790E-06	10.70	M151	2 1 2 2 2	
1.657E-08	3.783E-06	11.14	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.24	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.30	M082	1 1 1 2 2	
2.100E-08	4.794E-06	14.30	M151	2 1 2 2 2	
1.583E-08	3.613E-06	14.34	M183	1 2 1 1 2	
2.365E-08	5.400E-06	15	B385	0 0 0 0 0	
2.446E-08	5.584E-06	18.14	M183	1 2 1 1 2	
2.770E-08	6.324E-06	19.30	M082	1 1 1 2 2	
2.770E-08	6.324E-06	19.30	M151	2 1 2 2 2	
2.775E-08	6.335E-06	19.34	M183	1 2 1 1 2	
3.670E-08	8.378E-06	23.10	M082	1 1 1 2 2	
3.670E-08	8.378E-06	23.10	M151	2 1 2 2 2	
3.669E-08	8.377E-06	23.14	M183	1 2 1 1 2	
3.507E-08	8.007E-06	23.64	M183	1 2 1 1 2	
1.927E-07	4.400E-05	24	H116	2 1 0 0 1	
4.117E-08	9.400E-06	25	B319	2 0 1 2 1	
4.056E-08	9.260E-06	25	B385	0 0 0 0 0	
5.694E-08	1.300E-05	25	D406	1 2 2 2 2	
4.310E-08	9.840E-06	25	K001	2 2 2 2 2	
3.900E-09	8.904E-07	25	K123	1 0 2 2 1	*sic*
2.497E-08	5.700E-06	25	L332	1 1 1 1 2	
6.132E-08	1.400E-05	25	M064	1 1 2 2 1	
4.117E-08	9.400E-06	25	M071	2 2 2 2 2	
6.130E-08	1.399E-05	25	M342	1 0 1 1 2	
4.117E-08	9.400E-06	25.00	M151	2 1 1 2 1	
3.774E-08	8.617E-06	25.04	M183	1 2 1 1 2	
4.818E-08	1.100E-05	27	D003	1 0 0 1 1	

(*continued*)

3843. $C_{18}H_{12}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.344E-08	1.220E-05	29	M071	2 2 2 2 2	
5.344E-08	1.220E-05	29.00	M151	2 1 1 2 2	
5.436E-08	1.241E-05	29.54	M183	1 2 1 1 2	
5.580E-08	1.274E-05	29.70	M082	1 1 1 2 2	
5.580E-08	1.274E-05	29.70	M151	2 1 2 2 2	
5.567E-08	1.271E-05	29.74	M183	1 2 1 1 2	
7.635E-08	1.743E-05	35	B385	0 0 0 0 0	
6.132E-08	1.400E-05	ns	M344	0 0 0 0 2	

3844. $C_{18}H_{12}$

Chrysene

1,2-Benzphenanthrene

RN: 218-01-9 **MP** (°C)**:** 254

MW: 228.30 **BP** (°C)**:** 448

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-09	7.077E-07	6.50	M082	1 1 1 2 2	
3.100E-09	7.077E-07	6.50	M151	2 1 2 2 2	
3.500E-09	7.990E-07	11.00	M082	1 1 1 2 2	
3.500E-09	7.990E-07	11.00	M151	2 1 2 2 2	
6.130E-09	1.399E-06	20.40	M082	1 1 1 2 2	
6.130E-09	1.399E-06	20.40	M151	2 1 2 2 2	
6.139E-09	1.401E-06	20.44	M183	1 2 1 1 2	
9.199E-09	2.100E-06	23	P339	0 0 0 0 0	
7.446E-08	1.700E-05	24	H116	2 1 0 0 1	
7.360E-09	1.680E-06	24.00	M082	1 1 1 2 2	
7.360E-09	1.680E-06	24.00	M151	2 1 2 2 2	
7.367E-09	1.682E-06	24.04	M183	1 2 1 1 2	
4.818E-09	1.100E-06	25	B319	2 0 1 2 1	average of 2
6.570E-09	1.500E-06	25	D406	1 2 2 2 2	
2.760E-08	6.301E-06	25	K001	2 2 2 2 2	
2.628E-08	6.000E-06	25	L332	1 1 1 1 2	
8.761E-09	2.000E-06	25	M064	1 1 2 2 1	
7.884E-09	1.800E-06	25	M071	2 2 2 2 2	
8.760E-09	2.000E-06	25	M342	1 0 1 1 2	
7.884E-09	1.800E-06	25.00	M151	2 1 1 2 1	
8.280E-09	1.890E-06	25.30	M082	1 1 1 2 2	
8.280E-09	1.890E-06	25.30	M151	2 1 2 2 2	
8.283E-09	1.891E-06	25.34	M183	1 2 1 1 2	
6.570E-09	1.500E-06	27	D003	1 0 0 1 1	
9.680E-09	2.210E-06	28.70	M082	1 1 1 2 2	
9.680E-09	2.210E-06	28.70	M151	2 1 2 2 2	
9.689E-09	2.212E-06	28.74	M183	1 2 1 1 2	
9.637E-09	2.200E-06	29	M071	2 2 2 2 2	
9.637E-09	2.200E-06	29.00	M151	2 1 1 2 1	
8.761E-09	2.000E-06	ns	M344	0 0 0 0 2	
8.710E-09	1.988E-06	ns	R424	0 0 0 0 0	
3.400E-06	7.762E-04	ns	W005	0 0 1 2 1	*sic*

3845. $C_{18}H_{12}N_2$

2,2′-Biquinoline
2,2′-Biquinolyl
RN: 119-91-5 **MP** (°C)**:** 193
MW: 256.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-06	1.020E-03	24	H106	1 0 2 2 2	
3.980E-06	1.020E-03	24	M303	1 0 1 1 2	

3846. $C_{18}H_{12}N_4O$

4-Hydroxy-6,7-diphenylpteridine
4-Hydroxy-6:7-diphenylpteridine
RN: 102943-71-5 **MP** (°C)**:**
MW: 300.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-04	2.000E-01	20	A019	2 2 1 1 2	

3847. $C_{18}H_{13}ClFN_3$

Midazolam
8-Chloro-6-(*o*-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine
RN: 59467-70-8 **MP** (°C)**:**
MW: 325.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-04	5.400E-02	24	A404	2 0 2 2 2	intrinsic pH = 9.5

3848. $C_{18}H_{13}ClF_3NO_7$

Fluoroglycofen-ethyl
Super Blazer
Fluoroglycofen ethyl ester
Ethoxycarbonylmethyl-5-(2-chloro-4-trifluoromethylphenoxy)-2-nitrobenzoate-hyphen-ethoxy-2-oxoethyl 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoate
5-[2-Chloro-4-(trifluoromethyl)-phenoxy]-2-nitro-benzoic acid 2-ethoxy-2-oxoethyl ester
RN: 77501-90-7 **MP** (°C)**:**
MW: 447.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.349E-06	6.040E-04	ns	R427	0 0 0 0 0	

3849. $C_{18}H_{13}N$
6-Aminochrysene
6-Chrysenamine
RN: 2642-98-0 **MP** (°C)**:** 210
MW: 243.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-07	1.550E-04	24	H106	1 0 2 2 2	
6.370E-10	1.550E-07	ns	M349	0 2 1 1 2	

3850. $C_{18}H_{13}NO_3$
Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-6-methyl-1-phenyl-
RN: 74103-08-5 **MP** (°C)**:**
MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.463E-08	1.300E-05	25	P089	0 0 0 0 0	
1.270E-07	3.700E-05	37	P089	0 0 0 0 0	
2.163E-07	6.300E-05	51	P089	0 0 0 0 0	

3851. $C_{18}H_{13}NO_3$
N-1-Naphthylphthalamic acid
Naptalam
2-((1-Naphthylamino)carbonyl)benzoic acid
Naphthylphthalamic acid
ALANAP-1
NPA
RN: 132-66-1 **MP** (°C)**:** 185
MW: 291.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-04	2.000E-01	25	B200	1 0 0 0 2	
6.866E-04	2.000E-01	ns	B185	0 0 0 0 0	
6.866E-04	2.000E-01	ns	N013	0 0 0 0 2	
6.866E-04	2.000E-01	rt	M161	0 0 0 0 2	

3852. $C_{18}H_{14}$
o-Terphenyl
1,2-Diphenyl benzene
RN: 84-15-1 **MP** (°C)**:** 58
MW: 230.31 **BP** (°C)**:** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-06	1.239E-03	25	A325	2 1 2 2 2	

3853. $C_{18}H_{14}$
m-Terphenyl
1,3-Diphenyl benzene
RN: 92-06-8 **MP** (°C)**:** 89
MW: 230.31 **BP** (°C)**:** 365

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.560E-06	1.511E-03	25	A325	2 1 2 2 2	

3854. $C_{18}H_{14}$
p-Terphenyl
1,4-Diphenyl benzene
RN: 92-94-4 **MP** (°C)**:** 213
MW: 230.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-08	1.796E-05	25	A325	2 1 2 2 1	

3855. $C_{18}H_{14}Cl_4N_2O$
Miconazole
1-[2-(2,4-Dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1H-imidazole
1-[2,4-Dichloro-β-[(2,4-dichlorobenzyl)oxy]phenethyl]imidazole
Conoderm
RN: 22916-47-8 **MP** (°C)**:**
MW: 416.14 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.80E-09	<2.00E-06	25	P348	0 0 0 0 0	
2.163E-04	9.000E-02	amb	L434	0 0 0 0 0	

3856. $C_{18}H_{14}N_4O$
Disperse yellow 23
Phenol, 4-[[4-(phenylazo)phenyl]azo]-
p-Hydroxy-*p*-bis(azobenzene)
RN: 6250-23-3 **MP** (°C)**:**
MW: 302.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-10	6.047E-08	25	B333	0 0 0 0 0	
1.300E-07	3.930E-05	71.8	D093	1 2 1 2 0	EFG
5.500E-07	1.663E-04	84.1	D093	1 2 1 2 0	EFG
2.300E-06	6.954E-04	97.4	D093	1 2 1 2 0	EFG

3857. $C_{18}H_{14}N_4O_2$
Disperse orange 1
Dye VI
C.I. Disperse orange 1
4-(*p*-Nitrophenylazo)diphenylamine
4-Anilino-4′-nitroazobenzene
4-(4-Nitrophenylazo)diphenylamine
RN: 2581-69-3 **MP** (°C)**:** 157
MW: 318.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-09	4.775E-07	25	B333	0 0 0 0 0	
3.000E-07	9.550E-05	84.10	B198	1 2 1 1 0	
1.420E-06	4.520E-04	97.40	B198	1 2 1 1 2	
4.900E-06	1.560E-03	111.60	B198	1 2 1 1 1	
1.950E-05	6.208E-03	127	B198	1 2 1 1 2	

3858. $C_{18}H_{14}N_4O_5S$
Sulfasalazine
Salicylazosulfapyridine
SASP
Sulcolon
Salazosulfapyridine
Salicylazosulfapyridine
RN: 599-79-1 **MP** (°C)**:** 240–245
MW: 398.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.510E-05	1.000E-02	ns	K444	0 0 0 0 0	

3859. $C_{18}H_{15}Cl_3N_2O$
Econazole
1-[2-[(4-Chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]-1H-imidazole
RN: 27220-47-9 **MP** (°C)**:**
MW: 381.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-04	3.700E-01	amb	L434	0 0 0 0 0	

3860. $C_{18}H_{15}Cl_4N_3O_4$
Miconazole nitrate-β cyclidextrin complexant
RN: 22832-87-7 **MP** (°C)**:**
MW: 479.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-04	1.773E-01	25	P348	0 0 0 0 0	

3861. $C_{18}H_{15}NO_3$
Oxaprozin
4,5-Diphenyl-2-oxazolepropanoic acid
4,5-Diphenyl-2-oxazole-propionic acid
Choledyl
Daypro
Oxaprozin
RN: 21256-18-8 **MP** (°C)**:**
MW: 293.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.364E-05	4.000E-03	37	Y421	0 0 0 0 0	

3862. $C_{18}H_{15}N_3O_5$
1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, methyl ester
RN: 104663-14-1 **MP** (°C)**:** 156.5
MW: 353.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-05	7.000E-03	21	N337	0 0 0 0 0	pH 5
1.900E-05	6.713E-03	21	N337	0 0 0 0 0	pH 5

3863. $C_{18}H_{15}O_4P$
Triphenyl phosphate
Phosphoric acid triphenyl ester
Triphenyl phosphoric acid ester
Phenyl phosphate
TPP
RN: 115-86-6 **MP** (°C)**:** 49
MW: 326.29 **BP** (°C)**:** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.237E-06	7.300E-04	24	H116	2 1 0 0 2	
6.129E-05	2.000E-02	ns	F014	0 0 0 0 0	

3864. $C_{18}H_{16}ClNO_5$
Fenoxaprop-*p*-ethyl
Fenoxaprop-*p* ethyl ester
Propanoic acid
2-{4-{(6-Chloro-2-benzoxazolyl)oxy}phenoxy}-ethyl ester
RN: 71283-80-2 **MP** (°C)**:**
MW: 361.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-06	7.054E-04	ns	R427	0 0 0 0 0	

3865. $C_{18}H_{16}Cl_3N_3O_4$
Econazole nitrate
Pevaryl
Spectazole
R 14827
RN: 68797-31-9 **MP** (°C)**:**
MW: 444.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	7.115E-01	25	P348	0 0 0 0 0	

3866. $C_{18}H_{16}N_2O_3$
Benzoyltryptophan
N-Benzoyl-DL-tryptophan
RN: 2901-79-3 **MP** (°C)**:**
MW: 308.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-03	5.600E-01	25.1	N026	0 0 0 0 0	

3867. $C_{18}H_{16}N_4O_3S$
2-(*N*4-Acetylsulfanilylamino)-4-phenylpyrimidine
RN: **MP** (°C)**:**
MW: 368.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	3.600E-03	37	R076	1 2 0 0 1	

3868. $C_{18}H_{17}ClN_4O_6.0.5H_2O$
9-[5-*O*-(4-Chlorobenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)
RN: 121032-34-6 **MP** (°C)**:** 122–124
MW: 429.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-04	8.081E-02	37	M378	1 2 1 1 2	pH 7.2

3869. $C_{18}H_{17}Cl_2NO_3$
Benzoylprop-ethyl
Ethyl *N*-benzoyl-*N*-(3,4-dichlorophenyl)-2-aminopropionate
FX 2182
N-Benzoyl-*N*-(3,4-dichlorophenyl)-DL-alanine ethyl ester
Enaven
Suffix
RN: 22212-55-1 **MP** (°C)**:** 70.5
MW: 366.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.461E-05	2.000E-02	25	M161	1 0 0 0 1	

3870. $C_{18}H_{17}N_5O_8$
6-Methoxy-9-(5-*O*-[4-nitrobenzoyl]-β-D-arabinofuranosyl)-9H-purine
RN: 121032-21-1 **MP** (°C)**:** 202–203
MW: 431.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.467E-02	37	M378	1 2 1 1 2	pH 7.2

3871. $C_{18}H_{18}ClNO_4$
Clanobutin
Butanoic acid, 4-[(4-chlorobenzoyl)(4-methoxyphenyl)amino]-
Bykahepar
RN: 30544-61-7 **MP** (°C)**:**
MW: 347.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.270E-04	4.417E-02	37	K093	1 2 1 1 2	pH 3.0

3872. $C_{18}H_{18}ClNO_5$
Etofibrate
3-Pyridinecarboxylic acid, 2-[2-(4-chlorophenoxy)-2-methyl-1-oxopropoxy]ethyl ester
Tricerol
Lipo-Merz
RN: 31637-97-5 **MP** (°C)**:**
MW: 363.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.276E-03	rt	G093	0 1 1 1 2	pH4

3873. $C_{18}H_{18}ClNO_5$

Benzoximate

RN: 29104-30-1 **MP** (°C)**:** 73
MW: 363.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	3.026E-02	ns	R427	0 0 0 0 0	

3874. $C_{18}H_{18}ClNS$

Chlorprothixene
Taractan
1-Propanamine, 3-(2-chloro-9H-thioxanthen-9-ylidene)-*N*,*N*-dimethyl-, (3Z)-
Rentovet

RN: 113-59-7 **MP** (°C)**:**
MW: 315.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.936E-05	1.243E-02	20	H301	0 0 0 0 0	
1.221E-06	3.858E-04	22.5	B440	0 0 0 0 0	

3875. $C_{18}H_{18}N_2O_4$

C.I. Disperse blue 23
1,4-bis[(2-Hydroxyethyl)amino]anthraquinone
Acetoquinone blue BF

RN: 4471-41-4 **MP** (°C)**:** 248
MW: 326.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-06	7.833E-04	25	B333	0 0 0 0 0	

3876. $C_{18}H_{18}N_4O_6$

9-[5-*O*-(Benzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 121032-31-3 **MP** (°C)**:** 202–204
MW: 386.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-05	2.859E-02	37	M378	1 2 1 1 2	pH 7.2

3877. $C_{18}H_{18}N_4O_6.0.75H_2O$

2′-Benzoyl-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-44-6 **MP** (°C)**:** 84–86
MW: 399.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-02	7.118E+00	37	C348	0 0 0 0 0	pH 7.00

3878. $C_{18}H_{18}N_8O_6$

7,7′-Succinylditheophylline

RN: 58447-18-0 **MP** (°C)**:**
MW: 442.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-03	7.211E-01	25	L067	1 0 1 1 2	

3879. $C_{18}H_{18}O_2$

Dienestrol
3,4-bis(4-Hydroxyphenyl)-2,4-hexadiene
Dehydrostilbestrol

RN: 84-17-3 **MP** (°C)**:** 227.5
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-05	3.000E-03	37	B039	2 1 1 1 0	EFG
1.122E-05	2.988E-03	ns	R427	0 0 0 0 0	

3880. $C_{18}H_{18}O_2$

Equilenin
3-Hydroxy-17-keto-δ(1,3,5-10,6,8)estrapentaene
1,3,5-10,6,8-Estrapentaen-3-ol-17-one

RN: 517-09-9 **MP** (°C)**:** 258
MW: 266.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	1.520E-03	25	L033	1 0 2 1 2	

3881. $C_{18}H_{18}O_3$

Flurecol-butyl
Flurenol-*n*-butyl ester
n-Butyl-9-hydroxyfluorene-(9)-carboxylate
RN: 2314-09-2 **MP** (°C)**:** 70
MW: 282.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.293E-02	3.650E+00	20	B200	1 0 0 0 2	*sic*
1.293E-04	3.650E-02	20	M161	1 0 0 0 2	*sic*

3882. $C_{18}H_{19}Cl_2NO_4$

Felodipine
3,5-Pyridinedicarboxylic acid, 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-, ethyl methyl ester
Plendil
RN: 72509-76-3 **MP** (°C)**:**
MW: 384.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.301E-06	5.000E-04	20	N322	0 0 0 0 0	
1.179E-05	4.530E-03	22	M382	2 1 1 1 1	

3883. $C_{18}H_{19}F_3N_2S$

4-Trifluoromethyl-*N*,*N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 3852-94-6 **MP** (°C)**:**
MW: 352.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.467E-03	ns	G023	0 0 1 1 0	

3884. $C_{18}H_{19}F_3N_2S$

Fluopromazine
Triflupromazine
RN: 146-54-3 **MP** (°C)**:** <25
MW: 352.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.762E-03	24	G022	2 0 1 1 1	
5.000E-06	1.762E-03	ns	F027	0 0 0 0 0	

3885. $C_{18}H_{19}NO$
Desmethyldoxepin
1-Propanamine, 3-dibenz[b,e]oxepin-11(6H)-ylidene-*N*-methyl-
RN: 1225-56-5 **MP** (°C)**:**
MW: 265.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-04	1.048E-01	25	E051	1 0 2 1 2	

3886. $C_{18}H_{19}N_2O_4$
N-Benzoyl-L-tyrosinamide acetate
RN: **MP** (°C)**:**
MW: 327.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	4.256E-02	25	A066	1 0 1 1 1	

3887. $C_{18}H_{19}N_3O_6S$
Cephaloglycin
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
RN: 3577-01-3 **MP** (°C)**:**
MW: 405.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	1.050E+01	25	P311	0 0 0 0 0	EFG

3888. $C_{18}H_{19}N_5O_3$
C.I. Disperse dye
Propanenitrile, 3-[(2-hydroxyethyl)[3-methyl-4-[(4-nitrophenyl)azo]phenyl]amino]-
Celliton discharge scarlet RNL
Celliton fast scarlet RN
RN: 6054-58-6 **MP** (°C)**:** 156
MW: 353.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-07	6.714E-05	25	B333	0 0 0 0 0	

3889. $C_{18}H_{19}N_5O_6.0.3H_2O$
9-[5-*O*-(4-Aminobenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.3 hydrate)
RN: 121032-39-1 **MP** (°C)**:** 198–200
MW: 406.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.383E-02	37	M378	1 2 1 1 2	pH 7.2

3890. $C_{18}H_{19}N_5O_6$
2′-(*o*-Aminobenzoyl)-6-methoxypurine arabinoside
RN: 121032-55-1 **MP** (°C)**:**
MW: 401.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.060E-02	8.268E+00	37	C348	0 0 0 0 0	pH 7.00

3891. $C_{18}H_{20}$
2,4-Diphenyl-4-methyl-2-pentene
RN: 6362-80-7 **MP** (°C)**:**
MW: 236.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-07	2.475E-05	ns	D001	0 0 0 0 2	

3892. $C_{18}H_{20}Cl_2O_2$
1-Dichloro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 7388-32-1 **MP** (°C)**:**
MW: 339.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.664E-08	2.600E-05	rt	C122	0 0 0 0 0	

3893. $C_{18}H_{20}N_4O_7S$
2′-(*p*-Methylbenzenesulfonyl)-6-methoxypurine arabinoside
RN: 145913-49-1 **MP** (°C)**:** 214–215
MW: 436.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-04	5.412E-02	37	C348	0 0 0 0 0	pH 7.00

3894. $C_{18}H_{20}O_2$
Equilin
3-Hydroxy-17-keto-δ(1,3,5-10,7)estratetraene
1,3,5(10),7-Estratetraen-3-ol-17-one
RN: 474-86-2 **MP** (°C)**:** 238
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.217E-06	1.400E-03	25	H049	0 0 0 0 0	
5.254E-06	1.410E-03	25	L033	1 0 2 1 2	

3895. $C_{18}H_{20}O_2$
Diethylstilbestrol
Diethylstilboestrol
Destrol
4,4′-(1,2-Diethyl-1,2-ethenediyl)bisphenol
Tylosterone
Vagestrol
RN: 56-53-1 **MP** (°C)**:** 169
MW: 268.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-05	1.200E-02	25	G009	1 0 1 1 1	
9.316E-05	2.500E-02	30	M007	2 2 1 2 2	average of 6
		amb	L434	0 0 0 0 0	

3896. $C_{18}H_{21}ClN_2$
Chlorocyclizine
Chlorcyclizine
RN: 82-93-9 **MP** (°C)**:**
MW: 300.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	3.008E-01	37.5	L034	2 2 0 1 2	pH 7.4

3897. $C_{18}H_{21}ClN_2S$
2-Chloro-*N*,*N*-dimethyl-10H-phenothiazine-10-butanamine
RN: 13094-23-0 **MP** (°C)**:**
MW: 332.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.664E-03	ns	G023	0 0 1 1 0	

3898. $C_{18}H_{21}ClO$
1-Chloro-1-methyl-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane
RN: 56265-27-1 **MP** (°C)**:**
MW: 288.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.540E-06	1.600E-03	rt	C122	0 0 0 0 0	

3899. $C_{18}H_{21}NO_3$
Codeine
Codein
Methylmorphin
7,8-Didehydro-4,5-α-epoxy-3-methoxy-17-methylmorphinan-6-α-ol
Nucofed
Robitussin AC
RN: 76-57-3 **MP** (°C)**:** 155
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-02	9.000E+00	20	A073	1 1 1 1 0	
2.672E-02	8.000E+00	20	F300	1 0 0 0 0	
2.760E-02	8.264E+00	20	K052	1 1 1 1 2	
1.591E-01	4.762E+01	25	E041	2 2 2 2 0	EFG, form III, recrystallized
3.242E-02	9.705E+00	25	E041	2 2 2 2 0	EFG, form II, recrystallized
3.176E-02	9.509E+00	25	E041	2 2 2 2 0	EFG, form I, recrystallized
3.571E-02	1.069E+01	25	R338	0 0 0 0 0	
3.340E-02	1.000E+01	30	A073	1 1 1 1 1	
3.674E-02	1.100E+01	40	A073	1 1 1 1 1	
4.342E-02	1.300E+01	50	A073	1 1 1 1 1	
5.010E-02	1.500E+01	60	A073	1 1 1 1 1	
6.013E-02	1.800E+01	70	A073	1 1 1 1 1	
6.347E-02	1.900E+01	80	A073	1 1 1 1 1	
5.578E-02	1.670E+01	80	F300	1 0 0 0 2	
8.017E-02	2.400E+01	90	A073	1 1 1 1 1	
1.069E-01	3.200E+01	100	A073	1 1 1 1 1	

3900. $C_{18}H_{21}NO_3$
Thebainone A
Morphinan-6-one, 7,8-didehydro-4-hydroxy-3-methoxy-17-methyl-
Thebainon
RN: 467-98-1 **MP** (°C)**:** 146
MW: 299.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.000E+00	20	F300	1 0 0 0 0	
2.839E-02	8.500E+00	100	F300	1 0 0 0 1	

3901. $C_{18}H_{21}NO_3.H_2O$
Codeine (monohydrate)
Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, monohydrate, (5α,6α)
RN: 6059-47-8 **MP** (°C)**:** 155
MW: 317.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.604E-02	8.264E+00	c	D004	0 0 0 0 0	

3902. $C_{18}H_{21}NO_4$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(dimethylamino)-2-oxoethyl ester, (*S*)
Naproxen, *N*,*N*-dimethyl glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(dimethylamino)-2-oxoethyl ester
Naproxen *N*,*N*-dimethyl glycolamide ester
RN: 114665-18-8 **MP** (°C)**:** 150.5
MW: 315.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.268E-05	4.000E-03	21	B331	1 2 2 1 2	pH 7.4
1.268E-05	4.000E-03	21	B331	0 0 0 0 0	

3903. $C_{18}H_{22}ClNO_4$
Oxycodone hydrochloride
4,5-Epoxy-14-hydroxy-3-methoxy-17-methylmorphinan-6-one hydrochloride
Endocet
Percocet
Supeudol
Roxicet
RN: 124-90-3 **MP** (°C)**:** 270–271
MW: 351.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.060E-01	1.429E+02	ns	S469	0 0 0 0 0	

3904. $C_{18}H_{22}N_2$
1-(Diphenylmethyl)-4-methylpiperazine
RN: **MP** (°C)**:**
MW: 266.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.962E-04	1.855E-01	25	M438	0 0 0 0 0	

3905. $C_{18}H_{22}N_4O_5$
Dis. A. 9
Ethanol, 2,2′-[[4-[(2-methoxy-4-nitrophenyl)azo]-3-methylphenyl]imino]*bis*-
4-[bis(2-Hydroxyethyl)amino]-2′-methoxy-2-methyl-4′-nitroazobenzene
RN: 41541-11-1 **MP** (°C)**:**
MW: 374.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-06	1.685E-03	25	B333	0 0 0 0 0	

3906. $C_{18}H_{22}O_2$
Hexestrol
4,4′-(1,2-Diethylethylene)diphenol
Dihydrodiethylstilbestrol
Esestrolo
RN: 5635-50-7 **MP** (°C)**:** 186.5
MW: 270.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.438E-05	1.200E-02	37	B039	2 1 1 1 0	EFG
3.699E-05	1.000E-02	37	B045	1 0 1 1 1	
4.365E-05	1.180E-02	ns	R427	0 0 0 0 0	

3907. $C_{18}H_{22}O_2$
Estrone
Oestrone
Folliculin
1,3,5(10)-Estratrien-3-ol-17-one
Estra-1,3,5(10)-Trien-17-one, 3-hydroxy-
Oestrin
RN: 53-16-7 **MP** (°C)**:** 252.5
MW: 270.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.659E-06	1.530E-03	22	Y419	0 0 0 0 0	
2.959E-06	8.000E-04	25	H049	0 0 0 0 0	
1.110E-04	3.000E-02	25	I309	0 0 0 0 0	*sic*
2.959E-06	8.000E-04	25	L033	1 0 2 1 1	
1.109E-03	2.999E-01	25	P324	0 0 0 0 0	
4.808E-06	1.300E-03	25	S468	0 0 0 0 0	
8.200E-06	2.217E-03	37	H034	1 0 2 1 1	pH 7.4
1.184E-05	3.200E-03	37	L010	2 0 2 1 1	
3.162E-06	8.550E-04	ns	A074	0 0 0 0 0	EFG

3908. $C_{18}H_{23}NO$
Orphenadrine
Disipal
Marflex
Noradex
Orflagen
Norflex
RN: 83-98-7 **MP** (°C)**:**
MW: 269.39 **BP** (°C)**:** 195 at 12 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-06	1.801E-03	22.5	B440	0 0 0 0 0	

3909. $C_{18}H_{23}N_3O_3S$
L-Leu-dapsone
2-Amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-4-methyl-, (*S*)-
Pentanamide
RN: 160349-00-8 **MP** (°C)**:**
MW: 361.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.576E-04	3.100E-01	25	P351	0 0 0 0 0	pH 7.4
>6.92E-02	>2.50E+01	25	P351	0 0 0 0 0	

3910. $C_{18}H_{23}N_3O_4S$
Phentolamine methanesulfonate
Vasomax
Regitine mesylate
Regitine methanesulfonate
RN: 65-28-1 **MP** (°C)**:** 177
MW: 377.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.979E+00	1.502E+03	30	D011	1 0 1 0 2	

3911. $C_{18}H_{24}I_3N_3O_9$
1,3-Benzenedicarboxamide, 5*RS*-[(2,3-dihydroxy-1-oxobutyl)amino]-*N*,*N*′-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-[*RS*-(*RS**,*S**)]-
RN: 77868-48-5 **MP** (°C)**:**
MW: 807.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-01	1.071E+02	25	P091	0 0 0 0 0	

3912. $C_{18}H_{24}N_4O_2$
2,5-Diaziridinyl-3,6-dipyrrolidino-1,4-benzoquinone
RN: 59886-43-0 **MP** (°C)**:** 160
MW: 328.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.522E-03	5.000E-01	rt	C317	0 0 0 0 0	

3913. $C_{18}H_{24}N_4O_2S$
2-Sulfanilamido-5,6,7,8,-tetrahydro-8-isopropyl-5-methyl-quinazoline
RN: 71119-36-3 **MP** (°C)**:** 185-187
MW: 360.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-05	2.400E-02	29	C049	0 0 0 0 0	

3914. $C_{18}H_{24}N_4O_2S$
2-Sulfanilamidobornylenepyrimidine
RN: **MP** (°C)**:** 276
MW: 360.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.322E-05	3.000E-02	29	C049	0 0 0 0 0	

3915. $C_{18}H_{24}N_4O_3S$
L-Lys-dapsone
Hexanamide, 2,6-diamino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)
RN: 160349-03-1 **MP** (°C)**:**
MW: 376.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	pH 7.4
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	

3916. $C_{18}H_{24}O_2$
Estradiol
17-β-Estradiol
Estradiol-17β
RN: 50-28-2 **MP** (°C)**:** 176
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.652E-05	4.500E-03	20	G072	1 2 2 1 2	

(*continued*)

3916. $C_{18}H_{24}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.689E-03	20	L077	1 2 2 2 1	
1.413E-05	3.850E-03	22	Y419	0 0 0 0 0	
2.566E-05	6.990E-03	23	B014	0 0 1 2 2	
7.413E-06	2.019E-03	25	B041	1 0 2 2 0	EFG
6.000E-07	1.634E-04	25	E014	2 2 2 1 1	pH 7.3
1.432E-05	3.900E-03	25	H049	0 0 0 0 0	
1.836E-05	5.000E-03	25	K003	2 1 1 1 1	
5.544E-06	1.510E-03	25	S468	0 0 0 0 0	
1.320E-05	3.596E-03	27.34	L077	1 2 2 2 2	
2.060E-05	5.611E-03	35	L077	1 2 2 2 2	
1.500E-05	4.086E-03	37	H034	1 0 2 1 2	pH 7.4
2.350E-05	6.401E-03	37	H035	1 1 1 1 2	pH 7.4
1.430E-05	3.895E-03	37	H054	0 0 0 0 0	
1.880E-05	5.120E-03	37	R069	0 0 0 0 0	pH 7.4
1.000E-05	2.724E-03	37.50	B041	1 0 2 2 0	EFG
2.830E-05	7.709E-03	42	L077	1 2 2 2 2	
3.560E-05	9.697E-03	50	L077	1 2 2 2 2	

3917. $C_{18}H_{24}O_2$

α-Estradiol
17-α-Estradiol

RN: 57-91-0 **MP** (°C)**:** 220
MW: 272.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.432E-05	3.900E-03	25	L033	1 0 2 1 2	

3918. $C_{18}H_{24}O_3$

Estriol
Oestriol
Drihydroxyestrin

RN: 50-27-1 **MP** (°C)**:** 284.5
MW: 288.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	3.020E-02	22	Y419	0 0 0 0 0	
1.110E-05	3.200E-03	25	H049	0 0 0 0 0	
1.000E-04	2.884E-02	30	O321	0 0 0 0 0	
1.006E-04	2.900E-02	30	O321	0 0 0 0 0	

3919. $C_{18}H_{24}O_6$
Butylphthalyl butyl glycolate
1,2-Benzenedicarboxylic acid 2-butoxy-2-oxoethyl butyl ester
Butyl carbobutoxymethyl phthalate
RN: 85-70-1 **MP** (°C)**:** <–35
MW: 336.39 **BP** (°C)**:** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.567E-05	1.200E-02	20	F070	1 0 0 0 2	

3920. $C_{18}H_{25}I_3N_3O_9$
3,5-Diacetylamino-2,4,6-triiodobenzoic acid methyl-glucamide
RN: **MP** (°C)**:** 191
MW: 808.13 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.101E+00	8.900E+02	20	L100	1 0 0 0 1	

3921. $C_{18}H_{25}NO$
Racemethorphan
Dextromethorphan HBr
RN: 510-53-2 **MP** (°C)**:**
MW: 271.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-01	3.600E+01	37	F008	1 1 2 2 2	0.1N HCl

3922. $C_{18}H_{25}NO$
Dextromethorphan
(+)-*cis*-1,3,4,9,10,10a-Hexahydro-6-methoxy-11-methyl-2H-10,4a-iminoethanophenanthrene
Romilar CF
DXM Free Base
3-Methoxy-17-methyl-(9α,13α,14α)-morphinan
Benylin DM
RN: 125-71-3 **MP** (°C)**:**
MW: 271.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.316E-04	9.000E-02	amb	L434	0 0 0 0 0	

3923. $C_{18}H_{25}NO_5S_2$

Methyl *N*-{5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: **MP** (°C)**:**

MW: 399.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.003E-05	1.200E-02	ns	S453	0 0 0 0 0	

3924. $C_{18}H_{25}N_3O_2$

2-Ethoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide

N-[2-(Diethylamino)ethyl]-2-ethoxyquinoline-4-carboxamide

RN: 2716-99-6 **MP** (°C)**:**

MW: 315.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-04	2.082E-01	ns	M066	0 0 0 0 1	

3925. $C_{18}H_{26}NO_4$

Ibuprofen *N*-methyl-*N*-carbamoyl methyl glycolamide ester

RN: **MP** (°C)**:** 100.5

MW: 320.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.057E-04	1.300E-01	0	B331	1 2 2 1 1	pH 7.4

3926. $C_{18}H_{26}N_2O_4$

Benzeneacetic acid, β-methyl-4-(2-methylpropyl)-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxo-ethyl ester

Ibuprofen *N*-methyl-*N*-carbamoyl methyl glycolamide ester

RN: 114665-11-1 **MP** (°C)**:** 100–101

MW: 334.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	1.300E-01	21	B331	0 0 0 0 0	

3927. $C_{18}H_{26}N_4O_6$

9-[5-*O*-(Heptylate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 142963-79-9 **MP** (°C)**:** foam

MW: 394.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-04	8.362E-02	37	M378	1 2 1 1 2	pH 7.2

3928. $C_{18}H_{26}N_4O_6.0.5H_2O$

2′-Heptanyl-6-methoxypurine arabinoside (hemihydrate)
RN: 145913-40-2 **MP** (°C)**:** 83–85
MW: 403.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-03	1.122E+00	37	C348	0 0 0 0 0	pH 7.00

3929. $C_{18}H_{26}O$

Acetyl ethyl tetramethyl tetralin
1-(3-Ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)ethanone
AETT
1,1,4,4-Tetramethyl-6-ethyl-7-acetyl-1,2,3,4-tetrahydronaphthalene
Ethanone, 1-(3-ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl)-
RN: 88-29-9 **MP** (°C)**:**
MW: 258.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-08	1.200E-05	ns	B338	0 0 0 0 1	

3930. $C_{18}H_{26}O_2$

Nortestosterone
Estr-4-en-3-one, 17-hydroxy-, (17β)
RN: 434-22-0 **MP** (°C)**:**
MW: 274.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-02	3.090E+00	25	P324	0 0 0 0 0	

3931. $C_{18}H_{26}O_4$

Dipentyl phthalate
Diamyl phthalate
RN: 131-18-0 **MP** (°C)**:** <–55
MW: 306.41 **BP** (°C)**:** 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E-06	4.443E-04	20	L300	2 1 0 2 2	
9.791E-07	3.000E-04	25	F067	1 0 2 2 0	
3.263E-04	9.999E-02	ns	F014	0 0 0 0 0	

3932. $C_{18}H_{26}O_6$
Butyl phthalyl butyl glycollate
RN: **MP** (°C)**:**
MW: 338.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.955E-05	1.000E-02	15	H069	1 0 1 1 0	
5.318E-04	1.800E-01	ns	F014	0 0 0 0 1	

3933. $C_{18}H_{27}NO$
N-Nonylcinnamamide
2-Propenamide, *N*-nonyl-3-phenyl-
RN: 59832-01-8 **MP** (°C)**:**
MW: 273.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-06	6.070E-04	ns	H350	0 0 0 0 0	

3934. $C_{18}H_{27}NO_3$
p-Acetamidophenyl decanoate
Acetaminophen decanoate
RN: 54942-37-9 **MP** (°C)**:** 107
MW: 305.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.947E-05	9.000E-03	25	B010	1 1 1 1 0	

3935. $C_{18}H_{27}NO_3$
Capsaicin
Nonenamide, *N*-((4-hydroxy-3-methoxyphenyl)methyl)-8-methyl-, (E)-
Zostrix
RN: 404-86-4 **MP** (°C)**:** 63 C
MW: 305.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.176E-02	27	Z412	0 0 0 0 0	

3936. $C_{18}H_{27}N_5O_5$
9-[5′-(*O*-Caprylyl)-β-D-arabinofuranosyl]adenine ester
RN: 66460-51-3 **MP** (°C)**:**
MW: 393.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-04	1.000E-01	ns	B134	0 1 1 1 0	

3937. $C_{18}H_{28}N_2O$

DL-Bupivacaine
Bupivacaine
Marcaine
Bupivicaine
Marcaine (hydrochloride monohydrate)

RN: 2180-92-9 **MP** (°C)**:** 107
MW: 288.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	1.082E-01	14.9	N046	2 0 1 1 2	intrinsic
9.025E-06	2.603E-03	22.5	B440	0 0 0 0 0	
1.733E-03	5.000E-01	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
3.520E-04	1.015E-01	25	D401	1 2 2 2 2	
3.180E-04	9.172E-02	25	N046	2 0 1 1 2	intrinsic
3.130E-04	9.028E-02	34.5	N046	2 0 1 1 2	intrinsic
4.170E-04	1.203E-01	37	N044	2 1 1 2 2	intrinsic

3938. $C_{18}H_{28}N_4O_2$

2,5-Diaziridinyl-3,6-bis(butylamino)-1,4-benzoquinone

RN: 59886-48-5 **MP** (°C)**:** 95
MW: 332.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.01E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3939. $C_{18}H_{28}O_3$

Undecyl *p*-hydroxybenzoate
Undecyl 4-hydroxybenzoate

RN: 69679-31-8 **MP** (°C)**:**
MW: 292.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.079E-03	2.362E+00	25	D081	1 2 2 1 2	

3940. $C_{18}H_{29}NO_2$

Penbutolol
Levatol
2-Propanol, 1-(2-cyclopentylphenoxy)-3-[(1,1-dimethylethyl)amino]-, (*S*)-

RN: 38363-40-5 **MP** (°C)**:** 70
MW: 291.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.402E-02	7.000E+00	rt	H096	1 0 0 0 0	

3941. $C_{18}H_{29}NO_3$
4-Pentoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-73-8 **MP** (°C)**:**
MW: 307.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.845E-02	ns	M066	0 0 0 0 1	

3942. $C_{18}H_{30}$
2-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3943. $C_{18}H_{30}$
4-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3944. $C_{18}H_{30}$
5-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3945. $C_{18}H_{30}$
3-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	1.725E-06	25	S377	0 0 0 0 0	

3946. $C_{18}H_{30}$
6-Phenyldodecane
RN: **MP** (°C)**:**
MW: 246.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3947. $C_{18}H_{30}N_2O_2$
4-Pentylaminobenzoic acid-2-(diethylamino)ethyl ester
RN: 16488-56-5 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.435E-02	ns	M066	0 0 0 0 1	

3948. $C_{18}H_{30}O_3$
4-Octylphenol diethoxylate
2-[2-(*p*-Octylphenoxy)ethoxy]ethanol
RN: 51437-90-2 **MP** (°C)**:**
MW: 294.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.483E-05	1.320E-02	20.5	A335	0 0 0 0 0	
4.490E-05	1.322E-02	20.5	A335	0 0 0 0 0	

3949. $C_{18}H_{30}O_{15}.4H_2O$
Triamylose (tetrahydrate)
RN: **MP** (°C)**:**
MW: 558.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.298E-02	1.283E+01	20	P048	1 2 1 1 1	

3950. $C_{18}H_{31}NO_4$
Bisoprolol
1-[Isopropylamino]-3-[isopropoxyethoxymethylphenoxy]-2-propanol
ZEβ
Ziac
RN: 66722-44-9 **MP** (°C)**:**
MW: 325.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-08	5.500E-06	100	M418	0 0 0 0 0	

3951. $C_{18}H_{31}O_4P$

Butyl octyl phenyl phosphate

RN: 110459-55-7 **MP** (°C)**:**
MW: 342.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

3952. $C_{18}H_{32}O_7$

Tributyl citrate
Tri-*n*-butyl citrate
Butyl citrate

RN: 77-94-1 **MP** (°C)**:** –20
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.664E-04	6.000E-02	15	H069	1 0 1 1 0	
2.219E-04	7.999E-02	ns	F014	0 0 0 0 0	

3953. $C_{18}H_{32}O_{16}$

Raffinose
6G-α-D-Galactosylsucrose
Melitose
Gossypose
Melitriose

RN: 512-69-6 **MP** (°C)**:** 80.0
MW: 504.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.556E-02	3.307E+01	.02	H040	1 2 2 2 2	
1.227E-01	6.191E+01	10.00	H040	1 2 2 2 1	
1.879E-01	9.478E+01	16.38	H040	1 2 2 2 2	
1.937E-01	9.772E+01	16.90	H040	1 2 2 2 2	
2.480E-01	1.251E+02	20	D041	1 0 0 0 2	
2.373E-01	1.197E+02	20.00	H040	1 2 2 2 2	
3.192E-01	1.610E+02	24.80	H040	1 2 2 2 2	
4.555E-01	2.298E+02	25	P049	1 0 1 1 1	
3.228E-01	1.628E+02	25.05	H040	1 2 2 2 2	
3.340E-01	1.685E+02	25.50	H040	1 2 2 2 2	
4.227E-01	2.132E+02	30.00	H040	1 2 2 2 2	
6.398E-01	3.227E+02	39.38	H040	1 2 2 2 2	
6.599E-01	3.329E+02	40.00	H040	1 2 2 2 2	
9.217E-01	4.650E+02	50.00	H040	1 2 2 2 2	
1.016E+00	5.125E+02	53.20	H040	1 2 2 2 2	
1.201E+00	6.060E+02	60.00	H040	1 2 2 2 2	
1.239E+00	6.250E+02	61.60	H040	1 2 2 2 2	
1.473E+00	7.430E+02	70.00	H040	1 2 2 2 2	

(*continued*)

3953. $C_{18}H_{32}O_{16}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E+00	8.484E+02	78.00	H040	1 2 2 2 2	
6.518E-02	3.288E+01	.00	H040	1 2 2 2 1	
2.480E-01	1.251E+02	rt	D021	0 0 1 1 2	

3954. $C_{18}H_{32}O_{16}.5H_2O$

Raffinose (pentahydrate)
6G-α-D-Galactosylsucrose (pentahydrate)
RN: 17629-30-0 **MP** (°C)**:** 80
MW: 594.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.531E-02	3.288E+01	0	M043	1 0 0 0 1	
1.041E-01	6.191E+01	10	M043	1 0 0 0 1	
2.014E-01	1.197E+02	20	M043	1 0 0 0 2	
3.586E-01	2.132E+02	30	M043	1 0 0 0 2	
5.599E-01	3.329E+02	40	M043	1 0 0 0 2	
7.821E-01	4.650E+02	60	M043	1 0 0 0 2	
1.019E+00	6.060E+02	80	M043	1 0 0 0 2	

3955. $C_{18}H_{34}OSn$

Cyhexatin
Tricyclohexylhydroxystannane
Tricyclohexyltin hydroxide
Plictran
Dowco 213
RN: 13121-70-5 **MP** (°C)**:** 196.5
MW: 385.16 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.60E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.60E-06	<1.00E-03	ns	K138	0 0 0 0 1	

3956. $C_{18}H_{34}O_4$

Dibutyl sebacate
Di-*n*-butyl sebacate
Decanedioic acid dibutyl ester
Dibutyl decanedioate
RN: 109-43-3 **MP** (°C)**:**
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-04	5.000E-02	ns	F014	0 0 0 0 0	

3957. $C_{18}H_{36}O_2$

Stearic acid
Stearinsaeure
Octadecanoic acid

RN: 57-11-4 **MP** (°C)**:** 70
MW: 284.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.327E-06	1.800E-03	0	B136	1 0 2 1 1	
9.842E-06	2.800E-03	20	B136	1 0 2 1 1	
1.055E-05	3.000E-03	20	F300	1 0 0 0 0	
1.019E-05	2.900E-03	20.0	R001	1 1 1 1 1	
2.100E-06	5.974E-04	25	J001	1 0 2 1 1	
1.970E-06	5.604E-04	25	R002	0 0 0 0 0	
1.195E-05	3.400E-03	30	B136	1 0 2 1 1	
1.195E-05	3.400E-03	30.0	R001	1 1 1 1 1	
1.700E-05	4.836E-03	35	M004	2 0 0 0 2	
1.476E-05	4.200E-03	45	B136	1 0 2 1 1	
1.476E-05	4.200E-03	45.0	R001	1 1 1 1 1	
2.700E-06	7.681E-04	50	J001	1 0 2 1 1	
5.770E-05	1.641E-02	50	M004	2 0 0 0 2	
1.758E-05	5.000E-03	60	B136	1 0 2 1 1	
1.758E-05	5.000E-03	60	F300	1 0 0 0 0	
1.758E-05	5.000E-03	60.0	R001	1 1 1 1 1	
1.145E-05	3.257E-03	62.5	M004	1 0 0 0 2	
6.327E-06	1.800E-03	.0	R001	1 1 1 1 1	

3958. $C_{18}H_{38}$

n-Octadecane
Octadecane

RN: 593-45-3 **MP** (°C)**:** 29.5
MW: 254.50 **BP** (°C)**:** 317.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-07	1.200E-04	10	C331	0 0 0 0 0	
2.358E-08	6.000E-06	25	B069	1 0 1 1 1	
2.240E-08	5.700E-06	25	B069	1 0 1 1 1	
5.894E-07	1.500E-04	30	C331	0 0 0 0 0	
6.680E-07	1.700E-04	60	C331	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B003	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B033	0 0 0 0 2	

3959. $C_{18}H_{38}O$

Octadecanol
Stearyl alcohol
Octadecyl alcohol
Steraffine

RN: 112-92-5 **MP** (°C)**:** 61
MW: 270.50 **BP** (°C)**:** 336

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.082E-06	34	K011	1 2 1 1 1	
2.200E-08	5.951E-06	65	K011	1 2 1 1 1	

3960. $C_{18}H_{39}N.2H_2O$

Octadecylamine (dihydrate)
1-Aminooctadecane (dihydrate)

RN: 124-30-1 **MP** (°C)**:**
MW: 305.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.891E-09	1.800E-06	ns	R037	0 2 2 1 1	

3961. $C_{18}H_{39}O_3P$

Dibutyl decyl phosphonate

RN: 36378-71-9 **MP** (°C)**:**
MW: 334.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.00E-01	25	B070	1 2 0 1 0	

3962. $C_{18}H_{39}O_4P$

Dibutyl decyl phosphate

RN: 111440-78-9 **MP** (°C)**:**
MW: 350.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-04	<1.00E-01	25	B070	1 2 0 1 0	

3963. $C_{18}H_{39}O_7P$

Tributoxyethyl phosphate

RN: 78-51-3 **MP** (°C)**:** –70
MW: 398.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-03	1.100E+00	25	B070	1 2 0 1 1	

3964. $C_{19}H_{12}O_6$
Dicumarol
3,3′-Methylene-bis(4-hydroxycoumarin)
Dicoumarol
RN: 66-76-2 **MP** (°C)**:** 290
MW: 336.30 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.352E-05	1.800E-02	25	M457	0 0 0 0 0	
<4.46E-04	<1.50E-01	25	P312	0 0 0 0 0	

3965. $C_{19}H_{13}Cl$
6-Chloro-10-methyl-1,2-benzanthracene
RN: 188124-97-2 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.613E-08	1.000E-05	27	D003	1 0 0 1 0	

3966. $C_{19}H_{13}Cl$
4-Fluoro-10-methyl-1,2-benzanthracene
4-FMBA
RN: 2990-70-7 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3967. $C_{19}H_{13}Cl$
3-Fluoro-10-methyl-1,2-benzanthracene
3-FMBA
RN: 20629-50-9 **MP** (°C)**:**
MW: 276.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3968. $C_{19}H_{14}$
10-Methyl-1,2-benzanthracene
RN: 2541-69-7 **MP** (°C)**:** 141
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.539E-08	1.100E-05	24	H116	2 1 0 0 1	

3969. $C_{19}H_{14}$
1′-Methyl-1,2-benzanthracene
RN: 2498-77-3 **MP** (°C)**:** 138
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E-07	5.500E-05	27	D003	1 0 0 1 2	

3970. $C_{19}H_{14}$
5-Methylchrysene
RN: 3697-24-3 **MP** (°C)**:** 117.1
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-07	6.200E-05	27	D003	1 0 0 1 1	

3971. $C_{19}H_{14}$
9-Methyl-1,2-benzanthracene
RN: 2381-16-0 **MP** (°C)**:** 138
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.527E-07	3.700E-05	24	H116	2 1 0 0 1	

3972. $C_{19}H_{14}$
6-Methylchrysene
RN: 1705-85-7 **MP** (°C)**:** 149
MW: 242.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-07	6.500E-05	27	D003	1 0 0 1 1	

3973. $C_{19}H_{14}O_3$
Aurin
Rosolic acid
4-[*bis*-(*p*-Hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one
RN: 603-45-2 **MP** (°C)**:**
MW: 290.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-03	1.199E+00	rt	D021	0 0 1 1 1	

3974. $C_{19}H_{14}O_5S$
Phenolsulfonaphthalein
Phenolrot
RN: 143-74-8 **MP** (°C)**:** >300
MW: 354.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.748E-04	3.100E-01	100	F300	1 0 0 0 2	

3975. $C_{19}H_{16}O$
Triphenylcarbinol
Triphenylmethanol
RN: 76-84-6 **MP** (°C)**:** 164.2
MW: 260.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.432E+00	25	D007	2 0 1 1 2	

3976. $C_{19}H_{17}ClN_2O$
Prazepam
Centrax
7-Chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one
Demetrin
Verstran
RN: 2955-38-6 **MP** (°C)**:**
MW: 324.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	9.095E-03	25	M320	2 2 1 1 2	
		amb	L434	0 0 0 0 0	

3977. $C_{19}H_{17}ClN_2O_4$
Quizalofop-ethyl
Quizalofop-et
Quizalofop ethyl ester
Targa
Pilot
NC 302
RN: 76578-14-8 **MP** (°C)**:** 91.7–92.1
MW: 372.81 **BP** (°C)**:** 220 at 0.2 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.128E-07	3.030E-04	ns	R427	0 0 0 0 0	

3978. $C_{19}H_{17}ClN_2O_4$
Glafenine
N-(7-Chloro-4-quinolyl)anthranilate
2,3-Dihydroxypropyl-*N*-(7-chloro-4-quinolinyl)anthranilate
RN: 3820-67-5 **MP** (°C)**:** 169.5
MW: 372.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-01	3.846E+01	ns	M152	0 0 0 0 0	pH 1.0, intrinsic

3979. $C_{19}H_{17}ClN_4$
Fenbuconazole
α-(2-(4-Chlorophenyl)ethyl)-α-phenyl-1H-1,2,4-triazole-1-propanenitrile
Enable
RH-7592
Fenethanil
1,2,4-Triazole-1-propanenitrile, α-{2-(4-chlorophenyl)ethyl}-α-phenyl
RN: 114369-43-6 **MP** (°C)**:**
MW: 336.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-07	1.983E-04	ns	R427	0 0 0 0 0	

3980. $C_{19}H_{17}N_3O_4S_2$
Sugordomycin
RN: 1405-50-1 **MP** (°C)**:**
MW: 415.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.304E-02	9.572E+00	21	M044	2 0 2 2 2	

3981. $C_{19}H_{17}N_3O_4S_2$
Cephaloridine
Glaxoridin
Keflodin
Loridine
RN: 50-59-9 **MP** (°C)**:** 184
MW: 415.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.81E-02	>2.00E+01	21	M044	2 0 2 2 0	

3982. $C_{19}H_{17}N_3O_5$
1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, ethyl ester
RN: 153474-30-7 **MP** (°C)**:** 165.5
MW: 367.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.722E-05	1.000E-02	21	N337	0 0 0 0 0	pH 5
2.700E-05	9.919E-03	21	N337	0 0 0 0 0	pH 5

3983. $C_{19}H_{18}$
1,2,3,4-Tetrahydro-10-methyl-1,2-benzanthracene
10-Methyl-1,2-cyclohexane anthracene
RN: 6366-18-3 **MP** (°C)**:** 117
MW: 246.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.786E-07	4.400E-05	27	D003	1 0 0 1 1	

3984. $C_{19}H_{18}Cl_2N_2O_2$
G-20
p,*p*-Dichlorophenylbutazone
RN: 4047-57-8 **MP** (°C)**:**
MW: 377.27 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.386E-04	9.000E-02	ns	B158	0 0 0 0 1	pH 7.0

3985. $C_{19}H_{18}N_2O_3$
G-23
1-Oxybutylphenylbutazone
3,5-Pyrazolidinedione, 4-butyryl-1,2-diphenyl-
RN: 13167-98-1 **MP** (°C)**:**
MW: 322.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.722E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3986. $C_{19}H_{18}N_2O_3$
Kebuzone
3,5-Pyrazolidinedione
RN: 853-34-9 **MP** (°C)**:** 128
MW: 322.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.402E-04	1.742E-01	20	M140	2 0 1 1 1	

3987. $C_{19}H_{19}ClFNO_3$

Flamprop-isopropyl
Flufenprop-isopropyl
Isopropyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)alanine
1-Methylethyl *N*-benzoyl-*N*-(3-chloro-4-fluorophenyl)-DL-alanine
RN: 52756-22-6 **MP** (°C)**:** 56.5
MW: 363.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-05	1.800E-02	20	M161	1 0 0 0 0	

3988. $C_{19}H_{19}N_7O_6$

Folic acid
N-(*p*-(((2-Amino-4-hydroxy-6-pteridinyl)methyl)amino)benzoyl)-L-glutamic acid
Vitamin M
Pteroylglutamic acid
Folcysteine
Folacin
RN: 59-30-3 **MP** (°C)**:**
MW: 441.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-03	1.597E+00	25	D041	1 0 0 0 1	*sic*
3.625E-06	1.600E-03	25	D315	0 0 0 0 0	
2.243E-02	9.901E+00	100	D041	1 0 0 0 0	*sic*
2.265E-04	1.000E-01	ns	K444	0 0 0 0 0	

3989. $C_{19}H_{20}ClNO_9$

Griseofulvin-4-carboxy-methoxime
RN: **MP** (°C)**:**
MW: 441.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.704E-04	7.529E-02	37	F033	2 0 2 0 2	

3990. $C_{19}H_{20}F_3NO_4$

Fluazifop-butyl
Butyl 2-(4-((5-trifluoromethyl-2-pyridinyl)oxy)phenoxy)propanoate
Onecide
Fluazifop-butyl
Fluazifop butyl ester
Hache uno super
RN: 69806-50-4 **MP** (°C)**:** 13
MW: 383.37 **BP** (°C)**:** 165 at 2.02 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	5.366E-04	ns	S460	0 0 0 0 0	

3991. $C_{19}H_{20}N_2O$

Cinchoninone
Cinchoninon
9-Deoxy-9-oxocinchonine
RN: 14509-68-3 **MP** (°C)**:**
MW: 292.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.498E-04	1.900E-01	20	F300	1 0 0 0 1	

3992. $C_{19}H_{20}N_2O_2$

Phenylbutazone
1,2-Diphenyl-4-butyl-3,5-dioxopyrazolidine
Butazolidin
Equiphen
Butazone
RN: 50-33-9 **MP** (°C)**:** 107
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-05	2.595E-02	20	H301	0 0 0 0 0	
4.864E-05	1.500E-02	20	P026	1 0 1 1 1	
1.102E-04	3.400E-02	25	P096	0 0 0 0 0	
1.540E-04	4.750E-02	30	D015	2 0 1 1 0	EFG
1.000E-03	3.084E-01	35	H091	1 2 2 2 1	*sic*
9.076E-03	2.799E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
7.575E-03	2.336E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
9.362E-03	2.887E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
6.907E-03	2.130E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
2.108E-04	6.500E-02	37	D015	2 0 1 1 0	EFG
1.816E-04	5.600E-02	37	E047	1 0 1 1 1	
7.134E-03	2.200E+00	ns	B158	0 0 0 0 1	pH 7.0
1.037E-03	3.199E-01	ns	B404	0 2 1 1 0	
1.300E-04	4.009E-02	ns	O304	0 0 1 2 2	
2.594E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic
1.310E-01	4.040E+01	rt	N056	0 0 1 1 2	average of 2

3993. $C_{19}H_{20}N_2O_2$

G-21
p,*p*-Dimethylphenylbutazone
RN: 745-27-7 **MP** (°C)**:**
MW: 308.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.891E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3994. $C_{19}H_{20}N_2O_3$

Oxyphenbutazone
p-Hydroxyphenylbutazone
RN: 129-20-4 **MP** (°C)**:** 124
MW: 324.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	6.000E-02	30	D015	2 0 1 1 0	EFG
2.497E-04	8.100E-02	37	D015	2 0 1 1 0	EFG
3.083E-02	1.000E+01	ns	B158	0 0 0 0 1	pH 7.0, *sic*
>1.54E-03	>5.00E-01	ns	B404	0 2 1 1 0	
6.166E-05	2.000E-02	rt	H302	0 0 2 1 2	intrinsic

3995. $C_{19}H_{20}N_4O_6.0.5H_2O$

6-Methoxy-9-(5-*O*-[4-methylbenzoyl]-β-D-arabinofuranosyl)-9H-purine (hemihydrate)
RN: 121032-20-0 **MP** (°C)**:** 127–128
MW: 409.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-05	1.433E-02	37	M378	1 2 1 1 2	pH 7.2

3996. $C_{19}H_{20}N_4O_6$

2′-(*p*-Toluylyl)-6-methoxypurine arabinoside
2′-Phenylacetyl-6-methoxypurine arabinoside
RN: 121032-52-8 **MP** (°C)**:** 69–73
MW: 400.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.870E-02	2.350E+01	37	C348	0 0 0 0 0	pH 7.00
5.840E-03	2.338E+00	37	C348	0 0 0 0 0	pH 7.00

3997. $C_{19}H_{20}N_4O_6.0.1H_2O$

9-[5-*O*-(Benzyl formyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.1 hydrate)

RN: 121032-36-8 **MP** (°C)**:** foam
MW: 402.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-02	4.223E+00	37	M378	1 2 1 1 2	pH 7.2

3998. $C_{19}H_{20}N_4O_7$

2′-(*p*-Methoxybenzoyl)-6-methoxypurine arabinoside

RN: 121032-51-7 **MP** (°C)**:** 71–75
MW: 416.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-03	2.773E+00	37	C348	0 0 0 0 0	pH 7.00

3999. $C_{19}H_{20}N_4O_7.0.5H_2O$

2′-Phenoxyacetyl-6-methoxypurine arabinoside (hemihydrate)

RN: 145913-46-8 **MP** (°C)**:** 123–125
MW: 425.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.21E-02	>9.40E+00	37	C348	0 0 0 0 0	pH 7.00

4000. $C_{19}H_{20}N_4O_7.0.25H_2O$

9-[5-*O*-(4-Methoxybenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)

RN: 121032-35-7 **MP** (°C)**:** 195–197
MW: 420.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	8.250E-02	37	M378	1 2 1 1 2	pH 7.2

4001. $C_{19}H_{20}N_4O_7.0.05H_2O$

9-[5-*O*-(Benzyl acetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (0.05 hydrate)

RN: 121032-37-9 **MP** (°C)**:** 193-195
MW: 417.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.930E-04	1.640E-01	37	M378	1 2 1 1 2	pH 7.2

4002. $C_{19}H_{20}O_4$
Butylbenzyl phthalate
Butyl phenyl-methyl phthalate
Benzylbutyl phthalate
Phthalate butyl benzyl ester
Butyl benzyl phthalate
1,2-Benzenedicarboxylic acid butyl phenylmethyl ester
RN: 85-68-7 **MP** (°C)**:** <–35
MW: 312.37 **BP** (°C)**:** 370

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.020E-06	2.818E-03	20	L300	2 1 0 2 2	
3.778E-05	1.180E-02	22	Y419	0 0 0 0 0	
2.273E-06	7.100E-04	24	H116	2 1 0 0 2	
8.644E-06	2.700E-03	25	F067	1 0 2 2 1	

4003. $C_{19}H_{21}ClO_4$
Isobutyl (+/–)-2-[4-(4-chlorophenoxy)phenoxy]propionate
RN: 51337-71-4 **MP** (°C)**:** 39.5
MW: 348.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.160E-04	1.800E-01	22	M161	1 0 0 0 2	

4004. $C_{19}H_{21}F_3N_2S$
2-Trifluoromethyl-*N*,*N*-dimethyl-10H-phenothiazine-10-propanamide
RN: 2340-66-1 **MP** (°C)**:**
MW: 366.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.832E-03	ns	G023	0 0 1 1 0	

4005. $C_{19}H_{21}NO$
Doxepin
Adapin
Deptran
Sinequan
RN: 1668-19-5 **MP** (°C)**:** 120
MW: 279.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-04	3.157E-02	25	E051	1 0 2 1 2	

4006. $C_{19}H_{21}NO_3$
Thebaine
Paramorphine
Morphinan, 6,7,8,14-tetradehydro-4,5α-epoxy-3,6-dimethoxy-17-methyl-
RN: 115-37-7 **MP** (°C)**:**
MW: 311.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	6.850E-01	15	K059	2 2 2 0 1	

4007. $C_{19}H_{21}N_3O$
Zolpidem
RN: 82626-48-0 **MP** (°C)**:**
MW: 307.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.25E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4008. $C_{19}H_{21}N_5O_2$
Dis. A. 6
Propanenitrile, 3-[butyl[4-[(4-nitrophenyl)azo]phenyl]amino]-
RN: 69472-19-1 **MP** (°C)**:** 118
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-08	7.028E-06	25	B333	0 0 0 0 0	

4009. $C_{19}H_{21}N_5O_2$
Dye VII
4-[[(4-(*N*-Butyl-*N*-ethylnitrile)amino)phenyl]azo]nitrobenzene
RN: **MP** (°C)**:**
MW: 351.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-07	1.687E-04	71.80	B198	1 2 1 1 1	
9.700E-07	3.409E-04	84.10	B198	1 2 1 1 1	
2.020E-06	7.099E-04	97.40	B198	1 2 1 1 2	

4010. $C_{19}H_{21}N_5O_4$
Prazosin
Minipress
Pressin
RN: 19216-56-9 **MP** (°C)**:**
MW: 383.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.346E-06	3.200E-03	22.5	B422	0 0 0 0 0	

4011. $C_{19}H_{21}N_5O_5$
9-[5′-(*O*-Hydrocinnamoyl)-β-D-arabinofuranosyl]adenine ester
RN: 68325-41-7 **MP** (°C)**:**
MW: 399.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.756E-03	1.500E+00	ns	B134	0 1 1 1 1	

4012. $C_{19}H_{22}Cl_2O_2$
1-Methyl-1,1-dichloro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-23-7 **MP** (°C)**:**
MW: 353.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-07	5.000E-05	rt	C122	0 0 0 0 0	

4013. $C_{19}H_{22}N_2O$
Cinchonidine
Cinchonidin
(8α,9*R*)-Cinchonan-9-ol
L-Cinchonidine
RN: 485-71-2 **MP** (°C)**:** 210
MW: 294.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.650E-01	15	K059	2 2 2 0 0	
9.511E-05	2.800E-02	22	M459	0 0 0 0 0	
6.793E-04	2.000E-01	25	F300	1 0 0 0 0	
1.970E-03	5.800E-01	100	F300	1 0 0 0 1	
6.792E-04	2.000E-01	c	D004	0 0 0 0 0	
8.490E-04	2.499E-01	rt	D021	0 0 1 1 1	

4014. $C_{19}H_{22}N_2O$
Cinchonine
Cinchonan-9-ol
(+)-Cinchonine
(9S)-Cinchonan-9-ol
RN: 118-10-5 **MP** (°C)**:** 265
MW: 294.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-06	1.413E-03	15	K059	2 2 2 0 1	
2.378E-05	7.000E-03	22	M459	0 0 0 0 0	
9.253E-04	2.724E-01	25	D004	0 0 0 0 0	
9.171E-04	2.700E-01	100	F300	1 0 0 0 1	
8.150E-04	2.399E-01	rt	D021	0 0 1 1 1	

4015. $C_{19}H_{22}N_2OS$
Acetylpromazine
3-Acetyl-10-(3-dimethylaminopropyl)phenothiazine
Plegicil
Vetranquil
Notensil
Plivafen
RN: 61-00-7 **MP** (°C)**:**
MW: 326.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.901E-05	1.600E-02	25	L045	1 1 1 1 2	intrinsic

4016. $C_{19}H_{22}N_2O_5$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester
Naproxen *N*-methyl-*N*-carbamoyl methyl glycolamide ester
RN: 114681-69-5 **MP** (°C)**:** 179
MW: 358.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-04	5.900E-02	21	B331	0 0 0 0 0	

4017. $C_{19}H_{22}N_2S$
Mepazine
Pecazine
RN: 60-89-9 **MP** (°C)**:** 80
MW: 310.46 **BP** (°C)**:** 233

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-05	5.588E-03	24	G022	2 0 1 1 1	

4018. $C_{19}H_{23}ClO_2$
1-Chloro-1-methyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-22-6 **MP** (°C)**:**
MW: 318.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-06	8.800E-04	rt	C122	0 0 0 0 0	

4019. $C_{19}H_{23}NO_3$
Ethylmorphine
7,8-Didehydro-4,5-epoxy-3-ethoxy-17-methylmorphinan-6-ol
RN: 76-58-4 **MP** (°C)**:**
MW: 313.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.916E-03	2.794E+00	20	K052	1 1 1 1 2	

4020. $C_{19}H_{23}NO_4$
1-Methyl-1-nitro-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 26258-70-8 **MP** (°C)**:**
MW: 329.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.093E-06	3.600E-04	rt	C122	0 0 0 0 0	

4021. $C_{19}H_{23}NO_5$
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl ester
Naproxen *N*-methyl-*N*-ethanol glycolamide ester
RN: 114665-19-9 **MP** (°C)**:** 110
MW: 345.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.053E-04	1.400E-01	21	B331	0 0 0 0 0	

4022. $C_{19}H_{23}N_3$
Amitraz
1,5-Di(2,4-dimethylphenyl)-3-methyl-1,3,5-triazapenta-1,4-diene
Ovasyn
Mitac
Triazid
Baam
RN: 33089-61-1 **MP** (°C)**:** 86.5
MW: 293.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-06	1.000E-03	rt	M161	0 0 0 0 0	

4023. $C_{19}H_{23}N_3O_2$
Ergonovine
9,10-Didehydro-*N*-(2-hydroxy-1-methylethyl)-6-methylergoline-8-carboxamide
Ergometrine
RN: 60-79-7 **MP** (°C)**:**
MW: 325.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.21E+00	>3.94E+02	25	B443	0 0 0 0 0	

4024. $C_{19}H_{23}N_5O_4$
Benzoic acid, 4-[(dimethylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-68-6 **MP** (°C)**:**
MW: 385.43 **BP** (°C)**:** 651.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.373E-03	1.300E+00	21	B419	1 1 2 2 1	int

4025. $C_{19}H_{24}N_2$
1-(Diphenylmethyl)-4-ethylpiperazine
RN: **MP** (°C)**:**
MW: 280.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	5.693E-01	25	M438	0 0 0 0 0	

4026. $C_{19}H_{24}N_2$
Imipramine
10,11-Dihydro-*N*,*N*-dimethyl-5H-dibenz[b,f]azepine-5-propanamine
5-[3-(Dimethylamino)propyl]-10,11-dihydro-5H-dibenz[b,f]azepine
RN: 50-49-7 **MP** (°C)**:** 174
MW: 280.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.823E-02	24	G022	2 0 1 1 1	

4027. $C_{19}H_{24}N_2O$
Hydrocinchonine
Hydrocinchonin
Cinchotine
RN: 485-65-4 **MP** (°C)**:** 268
MW: 296.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.362E-03	7.000E-01	16	F300	1 0 0 0 1	
2.593E-03	7.686E-01	25	D004	0 0 0 0 0	

4028. $C_{19}H_{24}N_2OS$
Methotrimeprazine
Levomepromazine
RN: 60-99-1 **MP** (°C)**:** 117
MW: 328.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.089E-05	2.000E-02	25	A081	1 0 1 1 0	EFG

4029. $C_{19}H_{24}N_2O_2$
Praziquantel
2-Cyclohexyl-carbonyl-1,3,4,6,7,11b-hexahydro-2H-pyrazine(2,1-a)isoquinoline-4-one
Biltricide
Droncit
RN: 55268-74-1 **MP** (°C)**:**
MW: 312.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.812E-01	30	B402	2 0 1 1 0	EFG
1.280E-03	4.000E-01	ns	K444	0 0 0 0 0	

4030. $C_{19}H_{24}N_2O_2S$
Cyclohexyl-*p*-toluene sulfonamide
Cyclohexyl-4-toluene sulfonamide
RN: **MP** (°C)**:**
MW: 344.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-04	6.000E-02	ns	F014	0 0 0 0 0	

4031. $C_{19}H_{24}N_4O_7$
Propyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 420.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	1.387E-01	25	M316	1 1 1 1 2	

4032. $C_{19}H_{24}O$
1,1-Dimethyl-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane
RN: 56265-26-0 **MP** (°C)**:**
MW: 268.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-07	1.800E-04	rt	C122	0 0 0 0 0	

4033. $C_{19}H_{24}O_2$
1,1,1-Trimethyl-2,2-bis(*p*-methyloxylphenyl)ethane
RN: 4741-74-6 **MP** (°C)**:**
MW: 284.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.426E-06	6.900E-04	rt	C122	0 0 0 0 0	

4034. $C_{19}H_{24}O_3$
Adrenosterone
Androstene-3,11,17-trione
RN: 382-45-6 **MP** (°C)**:** 220
MW: 300.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.279E-04	9.849E-02	23.5	J003	2 0 2 1 2	average of 2
2.610E-04	7.840E-02	37	H004	0 0 0 0 0	
5.059E-04	1.520E-01	37	J003	1 0 2 1 2	

4035. $C_{19}H_{25}NO$

N,*N*-Dicyclopentylcinnamamide

2-Propenamide, *N*,*N*-dicyclopentyl-3-phenyl-

RN: 59832-08-5 **MP** (°C)**:**

MW: 283.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-07	2.196E-04	ns	H350	0 0 0 0 0	

4036. $C_{19}H_{26}I_3N_3O_{10}$

1,3-Benzenedicarboxamide, *N*,*N′*-bis[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-

RN: 77868-46-3 **MP** (°C)**:**

MW: 837.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-02	1.961E+01	25	P091	0 0 0 0 0	

4037. $C_{19}H_{26}N_6O_4S$

Benzenesulfonamide, 4-(1,3-diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-*N*-[2-(dimethylamino)ethyl]-

RN: 89073-49-4 **MP** (°C)**:** 264

MW: 434.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-04	1.100E-01	ns	H316	0 0 0 0 0	pH 7.4
2.647E-02	1.150E+01	ns	H316	0 0 0 0 0	0.1N HCL

4038. $C_{19}H_{26}O$

δ-4-Androstene-3-one

RN: **MP** (°C)**:**

MW: 270.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-06	<2.70E-04	25	E014	2 2 2 1 0	pH 7.3

4039. $C_{19}H_{26}O_2$
Androstenedione
4-Androstene-3,17-dione
Androst-4-en-3,17-dion
RN: 63-05-8 **MP** (°C)**:**
MW: 286.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.728E-02	25	E014	2 2 2 1 2	pH 7.3
2.840E-02	8.133E+00	25	P324	0 0 0 0 0	
1.399E-04	4.007E-02	37	H034	1 0 2 1 2	pH 7.4
1.700E-04	4.870E-02	37	L010	2 0 2 1 1	

4040. $C_{19}H_{27}N_3O$
Doxylamine ethanamine
RN: **MP** (°C)**:**
MW: 313.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	9.403E+00	37.5	L034	2 2 0 1 2	pH 7.4

4041. $C_{19}H_{27}N_3O_2$
2-Propoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-propoxyquinoline-4-carboxamide
RN: 2717-00-2 **MP** (°C)**:**
MW: 329.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-04	1.311E-01	ns	B018	0 0 0 0 2	
3.980E-04	1.311E-01	ns	M066	0 0 0 0 2	

4042. $C_{19}H_{28}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-undecyl ester
RN: 65267-95-0 **MP** (°C)**:**
MW: 375.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-05	7.420E-03	ns	M120	0 0 1 1 2	

4043. $C_{19}H_{28}N_4O_6$
2′-Octanyl-6-methoxypurine arabinoside
RN: 145913-41-3 **MP** (°C)**:** 75–77
MW: 408.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.110E-04	2.496E-01	37	C348	0 0 0 0 0	pH 7.00

4044. $C_{19}H_{28}O$
7α-Methyl-19-nortestosterone
Trestolone
19-Nor-7α-methyltestosterone
RN: 3764-87-2 **MP** (°C)**:**
MW: 272.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-04	9.200E-02	37	H004	0 0 0 0 0	

4045. $C_{19}H_{28}O_2$
Androstanedione
5α-Androstane-3,17-dione
RN: 846-46-8 **MP** (°C)**:** 142
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-04	3.290E-02	23.5	J003	1 0 2 1 2	average of 2
2.200E-04	6.346E-02	25	E014	2 2 2 1 2	pH 7.3
1.685E-04	4.860E-02	37	J003	1 0 2 1 2	average of 2

4046. $C_{19}H_{28}O_2$
Testosterone
17β-Hydroxyandrost-4-en-3-one
Halotensin
Virilon
Oreton
Testex
RN: 58-22-0 **MP** (°C)**:** 155
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-05	1.615E-02	10	B012	2 0 1 1 0	
6.390E-05	1.843E-02	10	L017	2 2 2 2 2	
2.254E-04	6.500E-02	15	F042	2 2 2 2 1	
7.550E-05	2.178E-02	15	L017	2 2 2 2 2	
7.900E-05	2.279E-02	20	B012	2 0 1 1 0	

(*continued*)

4046. $C_{19}H_{28}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.430E-04	7.009E-02	20	F012	1 0 1 1 1	
2.392E-04	6.900E-02	20	F042	2 2 2 2 1	
8.460E-05	2.440E-02	20	G072	1 2 2 1 2	
7.790E-05	2.247E-02	20	L017	2 2 2 2 2	
8.000E-05	2.307E-02	20	L070	1 2 0 2 0	EFG
6.870E-05	1.982E-02	20	L077	1 2 2 2 2	
8.000E-04	2.307E-01	20	L087	1 1 2 1 0	EFG
6.240E-05	1.800E-02	22.5	B422	2 0 2 2 2	
8.100E-05	2.336E-02	25	B012	2 0 1 1 0	
9.500E-05	2.740E-02	25	B041	1 0 2 2 1	
2.531E-04	7.300E-02	25	F042	2 2 2 2 1	
8.321E-05	2.400E-02	25	K003	2 1 1 1 1	
1.664E-04	4.800E-02	25	L009	1 0 0 1 1	
8.480E-05	2.446E-02	25	L017	2 2 2 2 2	
6.934E-05	2.000E-02	25	L338	1 0 1 1 2	
1.040E-04	3.000E-02	27.34	L077	1 2 2 2 2	
1.060E-04	3.057E-02	30	B012	2 0 1 1 0	
2.670E-04	7.700E-02	30	F042	2 2 2 2 1	
9.790E-05	2.824E-02	30	L017	2 2 2 2 2	
1.100E-04	3.173E-02	30	L068	1 0 0 1 0	EFG
2.500E-04	7.211E-02	30	L344	2 0 1 1 0	
1.040E-04	3.000E-02	30	M007	2 2 1 2 2	average of 8
8.876E-05	2.560E-02	30	T005	2 0 2 2 2	
1.096E-04	3.163E-02	31	A025	2 2 2 2 0	EFG
1.300E-04	3.750E-02	35	L017	2 2 2 2 2	
1.397E-04	4.029E-02	35	L077	1 2 2 2 2	
1.950E-04	5.624E-02	37	B013	1 0 2 2 0	average
1.250E-04	3.605E-02	37	E014	2 2 2 1 2	pH 7.3
1.013E-04	2.922E-02	37	H034	1 0 2 1 2	pH 7.4
1.259E-04	3.631E-02	37.50	B041	1 0 2 2 0	EFG
1.260E-04	3.634E-02	37.50	B041	1 0 2 2 2	
1.400E-04	4.038E-02	40	B012	2 0 1 1 0	
1.570E-04	4.528E-02	40	L017	2 2 2 2 2	
3.000E-04	8.653E-02	40	L070	1 2 0 2 0	EFG
1.702E-04	4.909E-02	42.34	L077	1 2 2 2 2	
1.870E-04	5.394E-02	45	L017	2 2 2 2 2	
2.100E-04	6.057E-02	50	B012	2 0 1 1 0	
2.350E-04	6.778E-02	50	L017	2 2 2 2 2	
2.053E-04	5.922E-02	50	L077	1 2 2 2 2	
6.795E-05	1.960E-02	ns	B057	0 2 1 1 2	
3.814E-05	1.100E-02	ns	B338	0 0 0 0 1	

4047. $C_{19}H_{28}O_2$
5,6-Dehydroisoandrosterone
Prasterone
Dehydroepiandrosterone
Dehydroisoandrosterone
RN: 53-43-0 **MP** (°C)**:** 140.5
MW: 288.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.558E-05	2.180E-02	23.5	J003	2 0 2 1 2	average of 6
1.000E-04	2.884E-02	37	E014	2 2 2 1 2	pH 7.3
1.040E-04	3.000E-02	37	H034	1 0 2 1 2	pH 7.4
1.144E-04	3.300E-02	37	J003	1 0 2 1 2	average of 4
8.633E-05	2.490E-02	ns	B057	0 2 1 1 2	

4048. $C_{19}H_{28}O_2.H_2O$
Testosterone (monohydrate)
Testosterone monohydrate -I
RN: 58-22-0 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.920E-02	15	F042	2 2 2 2 2	crystal-II
5.352E-05	1.640E-02	15	F042	2 2 2 2 2	crystal-I
7.081E-05	2.170E-02	20	F042	2 2 2 2 2	crystal-II
6.265E-05	1.920E-02	20	F042	2 2 2 2 2	crystal-I
8.256E-05	2.530E-02	25	F042	2 2 2 2 2	crystal-II
7.310E-05	2.240E-02	25	F042	2 2 2 2 2	crystal-I
9.333E-05	2.860E-02	30	F042	2 2 2 2 2	crystal-II
8.484E-05	2.600E-02	30	F042	2 2 2 2 2	crystal-I

4049. $C_{19}H_{28}O_3$
11-Ketoetiocholanolone
3α-Hydroxy-5β-androstane-11,17-dione
Etiocholanol-11-one
Ba 2684
RN: 739-27-5 **MP** (°C)**:**
MW: 304.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.269E-01	23	J003	2 0 2 1 2	average of 4
9.457E-04	2.879E-01	37	J003	1 0 2 1 2	average of 2

4050. $C_{19}H_{29}ClN_5O_6$
Terazosin
Hytrin
1-(4-Amino-6,7-dimethoxy-2-quinazolinyl)-4-((tetra-hydro-2-furanyl)carbonyl)-, monohydrochloride, dihydrate
(*RS*)-Piperazine
RN: 63590-64-7 **MP** (°C)**:**
MW: 458.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-05	3.060E-02	22.5	B440	0 0 0 0 0	

4051. $C_{19}H_{29}NO$
n-Decylcinnamamide
2-Propenamide, *N*-decyl-3-phenyl-
RN: 59832-02-9 **MP** (°C)**:**
MW: 287.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-06	7.272E-04	ns	H350	0 0 0 0 0	

4052. $C_{19}H_{29}NO$
Procyclidine
Kemadrin
RN: 77-37-2 **MP** (°C)**:**
MW: 287.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.669E-06	1.055E-03	22.5	B440	0 0 0 0 0	

4053. $C_{19}H_{29}N_5O_6$
9-(1,3-Dipivaloate-2-propoxymethyl)guanine
RN: 88110-72-9 **MP** (°C)**:** 231
MW: 423.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-05	7.000E-03	25	B360	0 0 0 0 0	

4054. $C_{19}H_{30}O$
Androstane-17-one
RN: 36378-49-1 **MP** (°C)**:** 119
MW: 274.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-07	<5.49E-05	25	E014	2 2 2 1 0	pH 7.3

4055. $C_{19}H_{30}OS$
Epitiostanol
RN: 2363-58-8 **MP** (°C)**:** 127
MW: 306.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.915E-06	1.200E-03	37	H120	1 1 1 1 1	normal saline

4056. $C_{19}H_{30}O_2$
Epiandrosterone
Isoandrosterone
RN: 481-29-8 **MP** (°C)**:** 161
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.955E-05	2.020E-02	23.5	J003	2 0 2 1 2	average of 5
8.160E-05	2.370E-02	37	J003	1 0 2 1 2	average of 3

4057. $C_{19}H_{30}O_2$
Androsterone
3α-Hydroxy-17-androstanone
3α-Hydroxy-5α-androstan-17-one
Hydroxy-5α-androstan-17-one
Epihydroxyetioallocholan-17-one
Hydroxy-17-androstanone
RN: 53-41-8 **MP** (°C)**:** 185
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-05	1.150E-02	23.5	J003	2 0 2 1 2	average of 2
4.300E-05	1.249E-02	37	E014	2 2 2 1 1	pH 7.3
6.163E-05	1.790E-02	37	J003	1 0 2 1 2	average of 2

4058. $C_{19}H_{30}O_2$
Stanolone
Androstanolone
RN: 521-18-6 **MP** (°C)**:** 181.0
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.185E+00	3.443E+02	ns	B057	0 2 1 1 2	

4059. $C_{19}H_{30}O_2$
Etiocholanolone
3α-Hydroxy-5β-androstane-17-one
5-Isoandrosterone
RN: 53-42-9 **MP** (°C)**:**
MW: 290.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.002E-04	2.910E-02	23.5	J003	2 0 2 1 2	average of 2
7.000E-05	2.033E-02	25	E014	2 2 2 1 1	pH 7.3, pyrogen

4060. $C_{19}H_{30}O_3$
p-(Dodecyloxy)benzoic acid
Dodecyl *p*-hydroxybenzoate
RN: 2312-15-4 **MP** (°C)**:** 95
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E-03	1.094E+00	25	D081	1 2 2 1 2	

4061. $C_{19}H_{30}O_3$
Androstane-3-β,11-β-diol-17-one
Hydroxyisoandrosterone
RN: 514-17-0 **MP** (°C)**:** 235
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.552E-04	7.819E-02	23.5	J003	1 0 2 1 2	average of 2

4062. $C_{19}H_{30}O_3$
11-Hydroxyetiocholanolone
5β-Androstan-17-one, 3α,11-dihydroxy-
RN: 3272-49-9 **MP** (°C)**:**
MW: 306.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	4.290E-02	23.5	J003	2 0 1 1 2	average of 2

4063. $C_{19}H_{31}NO_2$
Dodecyl *p*-aminobenzoate
p-Aminobenzoic acid dodecyl ester
RN: 20043-94-1 **MP** (°C)**:**
MW: 305.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-08	4.887E-06	37	F006	1 1 2 2 1	

4064. $C_{19}H_{31}NO_3$
4-Hexoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-74-9 **MP** (°C)**:**
MW: 321.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.286E-02	ns	M066	0 0 0 0 1	

4065. $C_{19}H_{31}NO_9$
Metoprolol tartrate
1-(Isopropylamino)-3-(*p*-(2-methoxyethyl)phenoxy)-2-propanol (2:1)
RN: 56392-17-7 **MP** (°C)**:**
MW: 417.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-01	4.300E+01	25	A412	1 0 2 2 1	int

4066. $C_{19}H_{32}$
2-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4067. $C_{19}H_{32}$
6-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4068. $C_{19}H_{32}$
5-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4069. $C_{19}H_{32}$
4-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4070. $C_{19}H_{32}$
3-Phenyltridecane
RN: **MP** (°C)**:**
MW: 260.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4071. $C_{19}H_{32}N_2O_2$
4-Hexylaminobenzoic acid-2-(diethyl-amino)ethyl ester
RN: 16488-57-6 **MP** (°C)**:**
MW: 320.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	6.089E-02	ns	M066	0 0 0 0 1	

4072. $C_{19}H_{32}O_3$
4-Nonylphenol diethoxylate
RN: 20427-84-3 **MP** (°C)**:**
MW: 308.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-05	3.640E-03	2	A335	0 0 0 0 0	
1.080E-05	3.331E-03	10	A335	0 0 0 0 0	
1.096E-05	3.380E-03	10	A335	0 0 0 0 0	
9.700E-06	2.992E-03	14	A335	0 0 0 0 0	
9.726E-06	3.000E-03	14	A335	0 0 0 0 0	
1.100E-05	3.393E-03	20.5	A335	0 0 0 0 0	
1.096E-05	3.380E-03	20.5	A335	0 0 0 0 0	
1.200E-05	3.702E-03	25	A335	0 0 0 0 0	
1.196E-05	3.690E-03	25	A335	0 0 0 0 0	

4073. $C_{19}H_{34}O_3$
Methoprene
Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate
Kabat
Precor
Dianex
Pharorid
RN: 40596-69-8 **MP** (°C)**:** 164
MW: 310.48 **BP** (°C)**:** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.477E-06	1.390E-03	25	D302	1 0 0 0 2	
6.442E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG

4074. $C_{19}H_{40}$
2,6,10,14-Tetramethylpentadecane
Pristane
RN: 1921-70-6 **MP** (°C)**:**
MW: 268.53 **BP** (°C)**:** 296

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.724E-11	1.000E-08	25	T423	0 0 0 0 0	

4075. $C_{20}H_9Cl_3F_5N_3O_3$

Chlorfluazuron
Atabron
Benzamide, *N*-[4-(3-chloro-5-trifluoromethyl-2-pyridinyl-oxy)-3,5-dichloro-phenyl-aminocarbonyl]-2,6-difluoro
Jupiter

RN: 71422-67-8 **MP** (°C)**:**
MW: 540.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-09	1.200E-06	20	M402	0 0 0 0 0	

4076. $C_{20}H_{12}$

Benzo(a)pyrene
1,2-Benzopyrene
3,4-Benzpyrene
Benzo[a]pyrene
Benz[a]pyrene

RN: 50-32-8 **MP** (°C)**:** 179
MW: 252.32 **BP** (°C)**:** 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.309E-09	8.350E-07	15	B385	0 0 0 0 0	
2.000E-09	5.046E-07	20	E009	1 0 0 0 1	
2.972E-05	7.500E-03	23	T025	1 2 0 1 1	*sic*
6.341E-09	1.600E-06	25	B319	2 0 1 2 1	
5.667E-09	1.430E-06	25	B385	0 0 0 0 0	
7.213E-09	1.820E-06	25	D406	1 2 2 2 2	
4.400E-10	1.110E-07	25	K123	1 0 2 2 1	
1.506E-08	3.800E-06	25	L332	1 1 1 1 2	
1.506E-08	3.800E-06	25	M064	1 1 2 2 1	
1.500E-08	3.785E-06	25	M342	1 0 1 1 1	
6.428E-09	1.622E-06	25.04	M183	1 2 1 1 2	
1.585E-08	4.000E-06	27	D003	1 0 0 1 1	
9.083E-09	2.292E-06	30.04	M183	1 2 1 1 2	
1.098E-08	2.770E-06	35	B385	0 0 0 0 0	
1.506E-08	3.800E-06	ns	M344	0 0 0 0 2	
2.400E-08	6.056E-06	ns	W005	0 0 1 2 1	
4.756E-09	1.200E-06	ns	W302	0 0 0 0 1	

4077. $C_{20}H_{12}$
Benzo(k)fluoranthene
11,12-Benzo[k]fluoranthene
11,12-Benzofluoranthene
8,9-Benzofluoranthene
2,3,1′,8′-Binaphthylene
B[K]F
RN: 207-08-9 **MP** (°C)**:** 216
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-09	1.090E-06	25	D406	1 2 2 2 2	
3.171E-09	8.000E-07	ns	W302	0 0 0 0 0	

4078. $C_{20}H_{12}$
Benzo(j)fluoranthene
Benzo[l]fluoranthene
Benzo-12,13-fluoranthene
10,11-Benzofluoranthene
RN: 205-82-3 **MP** (°C)**:** 165
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.908E-09	2.500E-06	ns	W302	0 0 0 0 1	

4079. $C_{20}H_{12}$
Benzo(e)pyrene
4,5-Benzopyrene
B[E]P
RN: 192-97-2 **MP** (°C)**:** 178.5
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-09	9.840E-07	25	K123	1 0 2 2 1	
~1.59E-08	~4.00E-06	25	S227	1 2 1 1 0	
6.625E-02	1.672E+01	318	S355	1 1 1 2 0	EFG
1.192E-01	3.007E+01	330	S355	1 1 1 2 0	EFG
1.524E-01	3.846E+01	335	S355	1 1 1 2 0	EFG
2.066E-01	5.213E+01	342	S355	1 1 1 2 0	EFG
4.246E-01	1.071E+02	361	S355	1 1 1 2 0	EFG
4.559E-01	1.150E+02	365	S355	1 1 1 2 0	EFG

4080. $C_{20}H_{12}$
Perylene
Dibenz[de,kl]anthracene
peri-Dinaphthalene
RN: 198-55-0 **MP** (°C)**:** 273
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-10	1.060E-07	20	E009	1 0 0 1 1	
1.585E-09	4.000E-07	25	M064	1 1 2 2 0	
1.600E-09	4.037E-07	25	M342	1 0 1 1 1	
<1.98E-09	<5.00E-07	27	D003	1 0 0 1 0	
1.585E-09	4.000E-07	ns	M344	0 0 0 0 1	

4081. $C_{20}H_{12}$
Benzo(b)fluoranthene
3,4-Benzofluoranthene
2,3-Benzofluoranthene
B[B]F
RN: 205-99-2 **MP** (°C)**:** 108
MW: 252.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.945E-09	1.500E-06	ns	W302	0 0 0 0 1	

4082. $C_{20}H_{13}N$
13H-Dibenzo(a,i)carbazole
1:2,7:8-Dibenzocarbazole
RN: 239-64-5 **MP** (°C)**:** 220
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.00E-08	<1.34E-05	22	B175	1 0 1 1 0	*sic*
3.890E-08	1.040E-05	24	H106	1 0 2 2 2	
3.890E-08	1.040E-05	24	M303	1 0 1 1 2	

4083. $C_{20}H_{13}N$
3,4,5,6-Dibenzocarbazole
3:4,5:6-Dibenzocarbazole
RN: 194-59-2 **MP** (°C)**:** 158
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-07	5.347E-05	22	B175	1 0 1 1 0	

4084. $C_{20}H_{13}N$
1,2,5,6-Dibenzocarbazole
1:2,5:6-Dibenzocarbazole
RN: 207-84-1 **MP** (°C)**:**
MW: 267.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.337E-05	22	B175	1 0 1 1 0	

4085. $C_{20}H_{14}$
3,4′-Ace-1,2-benzanthracene
Benz[k]acephenanthrene
RN: 5779-79-3 **MP** (°C)**:**
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-08	2.700E-06	27	D003	1 0 0 1 1	

4086. $C_{20}H_{14}$
Cholanthrene
1,2-Dihydroxybenz[j]aceanthrylene
RN: 479-23-2 **MP** (°C)**:** 173
MW: 254.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.376E-08	3.500E-06	27	D003	1 0 0 1 1	

4087. $C_{20}H_{14}I_6N_2O_6$
Di(3-carboxy-2,4,6-triiodoanilido)adipic acid
Iodipamide
RN: 606-17-7 **MP** (°C)**:** 306
MW: 1139.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-04	4.600E-01	20	N035	1 1 2 1 1	
>4.38E-04	>5.00E-01	ns	B404	0 2 1 1 0	
1.404E-04	1.600E-01	ns	H055	0 0 0 0 0	

4088. $C_{20}H_{14}N_2O_2$
Disperse blue 19
C.I. Disperse blue 19
RN: 4395-65-7 **MP** (°C)**:** 194
MW: 314.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-10	1.918E-07	25	B333	0 0 0 0 0	
2.100E-07	6.601E-05	60.0	D093	1 2 1 2 0	EFG
5.000E-07	1.572E-04	71.8	D093	1 2 1 2 0	EFG
1.700E-06	5.344E-04	81.4	D093	1 2 1 2 0	EFG
4.200E-06	1.320E-03	97.4	D093	1 2 1 2 0	EFG

4089. $C_{20}H_{14}O_2$
3,3-Diphenylphthalide
3,3-Diphenyl-phthalid
RN: 596-29-2 **MP** (°C)**:**
MW: 286.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	4.000E-02	25	F300	1 0 0 0 0	

4090. $C_{20}H_{14}O_4$
Phenolphthalein
2-[bis(4-Hydroxyphenyl)methyl]benzoic acid
Espotabs
Alophen
Figsen
Laxettes
RN: 77-09-8 **MP** (°C)**:** 260.0
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.000E-03	25	H064	1 2 2 0 2	
7.476E-04	2.380E-01	100	H064	1 2 2 0 2	
1.256E-03	3.998E-01	rt	D021	0 0 1 1 0	

4091. $C_{20}H_{14}O_4$
Phenyl phthalate
Diphenyl phthalate
RN: 84-62-8 **MP** (°C)**:** 71
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.576E-07	8.200E-05	24	H116	2 1 0 0 1	

4092. $C_{20}H_{14}O_4$
Diphenyl *o*-phthalate
RN: **MP** (°C)**:** 72 C
MW: 318.33 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.424E-06	3.000E-03	25	S417	0 0 0 0 0	

4093. $C_{20}H_{15}O_5P$
bis(4-Carboxyphenyl)phenylphosphine oxide
BCPPO
RN: 803-19-0 **MP** (°C)**:**
MW: 366.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	7.326E-02	23	W402	0 0 0 0 0	
3.166E-04	1.160E-01	32	W402	0 0 0 0 0	
4.666E-04	1.709E-01	40	W402	0 0 0 0 0	
6.943E-04	2.543E-01	50	W402	0 0 0 0 0	
1.011E-03	3.702E-01	60	W402	0 0 0 0 0	
1.638E-03	6.000E-01	70	W402	0 0 0 0 0	
1.987E-03	7.280E-01	75	W402	0 0 0 0 0	

4094. $C_{20}H_{16}$
5,6-Dimethylchrysene
Chrysene, 5,6-dimethyl-
RN: 3697-27-6 **MP** (°C)**:** 127
MW: 256.35 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.752E-08	2.500E-05	27	D003	1 0 0 1 1	

4095. $C_{20}H_{16}$
9,10-Dimethyl-1,2-benzanthracene
7,12-Dimethyl-1,2-benzanthracene
7,12-Dimethylbenz[a]anthracene
9,10-Dimethyl-benz[a]anthracene
RN: 56-56-4 **MP** (°C)**:** 122
MW: 256.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.518E-08	2.440E-05	24	H106	1 0 2 2 2	
2.145E-07	5.500E-05	24	H116	2 1 0 0 1	
9.752E-08	2.500E-05	24	M129	1 2 1 1 1	
2.380E-07	6.100E-05	25	M064	1 1 2 2 1	
9.518E-08	2.440E-05	25	M156	1 2 1 1 2	
1.677E-07	4.300E-05	27	D003	1 0 0 1 1	

4096. $C_{20}H_{16}$
10-Ethyl-1,2-benzanthracene
10-Ethylbenz[a]anthracene
RN: 14854-08-1 **MP** (°C)**:** 114
MW: 256.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.755E-07	4.500E-05	27	D003	1 0 0 1 1	
1.560E-07	4.000E-05	27	D043	2 0 0 0 0	average of 2

4097. $C_{20}H_{16}O_4$
Phenolphthalin
Benzoic acid, 2-[bis(4-hydroxyphenyl)methyl]-
RN: 81-90-3 **MP** (°C)**:** 237
MW: 320.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.463E-04	1.750E-01	20	F300	1 0 0 0 2	

4098. $C_{20}H_{17}FO_3S$
Sulindac
Aclin
Clinoril
Clusinol
Saldac
RN: 38194-50-2 **MP** (°C)**:**
MW: 356.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-05	7.000E-03	37	Y421	0 0 0 0 0	

4099. $C_{20}H_{18}O_2Sn$
Triphenyltin hydroxide acetate
Fentin acetate
RN: 900-95-8 **MP** (°C)**:** 120
MW: 409.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.845E-05	2.800E-02	20	M161	1 0 0 0 1	

4100. $C_{20}H_{18}O_{10}$
Biphenyl dimethyl dicarboxylate
DDB
RN: **MP** (°C)**:**
MW: 418.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E-05	4.200E-03	ns	K446	0 0 0 0 0	

4101. $C_{20}H_{19}NO_3$
Acronine
3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano(2,3-c)acridin-7-one
Acronycine
RN: 7008-42-6 **MP** (°C)**:** 175–176
MW: 321.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.779E-06	2.500E-03	22	B064	1 0 1 1 0	
8.401E-06	2.700E-03	25	R071	0 0 0 0 0	

4102. $C_{20}H_{19}NO_5.6H_2O$
Berberine (hexahydrate)
Berberine
RN: 2086-83-1 **MP** (°C)**:** 145dec
MW: 461.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.422E-02	4.348E+01	25	D004	0 0 0 0 0	

4103. $C_{20}H_{19}N_3$
Rosaniline
Basic violet 14
C.I. 42510
Calcozine magenta xx
Cerise B
RN: 632-99-5 **MP** (°C)**:**
MW: 301.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.951E-04	2.999E-01	rt	D021	0 0 1 1 0	

4104. $C_{20}H_{19}N_3O_5$

1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, propyl ester

RN: 153474-31-8 **MP** (°C)**:** 113.5
MW: 381.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5

4105. $C_{20}H_{20}ClNO_7$

BTA-243

1,3-Benzodioxole-2,2-dicarboxylic acid, 5-[2-[[2-(3-chlorophenyl)-2-hydroxyethyl]amino] propyl]-

RN: **MP** (°C)**:**
MW: 421.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.890E-03	3.750E+00	25	B421	0 0 1 1 0	Zwitterion, EFG

4106. $C_{20}H_{20}N_2O_6$

Succinyl acetaminophen

Butanedioic acid, bis[4-(acetylamino)phenyl] ester

Acetanilide, 4′-hydroxy-, succinate

Acetanilide, 4′-hydroxy-, succinate (2:1) (ester)

RN: 2725-63-5 **MP** (°C)**:** 229–230
MW: 384.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.769E-05	6.800E-03	37	D029	0 0 0 0 0	

4107. $C_{20}H_{20}N_6O_6S_2$

2,5-Di-(*N*4-acetylsulfanilylamino)pyrimidine

RN: **MP** (°C)**:**
MW: 504.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.910E-06	5.000E-03	37	R076	1 2 0 0 1	

4108. $C_{20}H_{21}ClO_4$
Fenofibrate
Proctofene
Sedufen
RN: 49562-28-9 **MP** (°C)**:**
MW: 360.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E-06	8.000E-04	25	J415	0 0 0 0 0	

4109. $C_{20}H_{21}NO_4$
Papaverine
Pantoyl taurine
RN: 58-74-2 **MP** (°C)**:** 147
MW: 339.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.733E-02	37.5	L034	2 2 0 1 2	pH 7.4

4110. $C_{20}H_{21}NO_5$
Aspirin phenylalanine ethyl ester
L-Phenylalanine, *N*-[2-(acetyloxy)benzoyl]-, ethyl ester
RN: 76748-72-6 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	1.670E-01	25	B182	2 2 1 1 1	

4111. $C_{20}H_{21}NO_5$
Repirinast
Isoamyl 5,6-dihydro-7,8-dimethyl-4,5-dioxo-4H-pyrano(3,2-c)quinoline-2-carboxylate
RN: 73080-51-0 **MP** (°C)**:**
MW: 355.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-06	1.200E-03	ns	S470	0 0 0 0 0	

4112. $C_{20}H_{22}ClN$
Pyrrobutamine
Pyrrolidine, 1-[4-(4-chlorophenyl)-3-phenyl-2-butenyl]-
RN: 91-82-7 **MP** (°C)**:**
MW: 311.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	2.713E-01	37.5	L034	2 2 0 1 2	pH 7.4

4113. $C_{20}H_{22}FN_3O_7$
3-Quinolinecarboxylic acid
7-[4-[[(acetyloxy)methoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-
RN: 99106-30-6 **MP** (°C)**:**
MW: 435.41 **BP** (°C)**:** 636.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.445E-04	1.500E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.378E-04	6.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
6.890E-05	3.000E-02	25	A414	1 0 1 1 1	pH 5 phosphate buffer (0.1 M)

4114. $C_{20}H_{22}N_2O_2$
Quininone
Chininon
Cinchonan-9-one, 6′-methoxy-, (8α)-
RN: 84-31-1 **MP** (°C)**:** 212
MW: 322.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.305E-06	3.000E-03	20	F300	1 0 0 0 0	

4115. $C_{20}H_{22}N_8O_5$
Methotrexate
(+)-4-Amino-10-methylfolic acid
Metatrexan
Methoblastin
Maxtrex
Ledertrexate
RN: 59-05-2 **MP** (°C)**:** 195
MW: 454.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.290E+00	1.950E+03	c	B443	0 0 0 0 0	
2.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4116. $C_{20}H_{23}N$
Maprotiline
Maprotyline
RN: 10262-69-8 **MP** (°C)**:**
MW: 277.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	8.334E-04	22.5	B440	0 0 0 0 0	

4117. $C_{20}H_{23}NO_2$
Dexoxadrol
(+)-2-(2,2-Diphenyl-1,3-dioxolan-4-yl)piperidine
Relane
CL 911C
RN: 4741-41-7 **MP** (°C)**:**
MW: 309.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	7.000E-02	rt	K017	0 2 2 2 2	intrinsic

4118. $C_{20}H_{23}N_7O_7$
*N*5-Formyltetrahydropteroylglutamic acid
RN: 58-05-9 **MP** (°C)**:**
MW: 473.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.85E+00	>1.35E+03	25	B443	0 0 0 0 0	

4119. $C_{20}H_{24}ClN_3S$
Prochlorperazine
Compazine
Ultrazine
Cotranzine
Compa-Z
RN: 58-38-8 **MP** (°C)**:** 228
MW: 373.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.496E-02	24	G022	2 0 1 1 1	

4120. $C_{20}H_{24}N_2$
Dimethindene
Dimetindene
Pyridine, 2-[1-[2-[2-(dimethylamino)ethyl]inden-3-yl]ethyl]-
RN: 5636-83-9 **MP** (°C)**:**
MW: 292.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.160E-04	2.386E-01	37	L094	2 0 0 1 2	pH>10.03, intrinsic

4121. $C_{20}H_{24}N_2O_2$
Quinine
Chinin
Quinine alkaloid
RN: 130-95-0 **MP** (°C)**:** 177
MW: 324.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E-03	5.000E-01	15	F300	1 0 0 0 0	
9.555E-05	3.100E-02	22	M459	0 0 0 0 0	
1.760E-03	5.711E-01	25	D004	0 0 0 0 0	
9.247E-04	3.000E-01	25	P015	0 0 0 0 0	
4.007E-03	1.300E+00	100	F300	1 0 0 0 1	
<3.08E-04	<1.00E-01	rt	B435	0 0 0 0 0	
1.756E-03	5.697E-01	rt	D021	0 0 1 1 1	

4122. $C_{20}H_{24}N_2O_2$
Quinidine
Chinidin
Cinchonan-9-ol, 6′-methoxy-, (9*S*)-
RN: 56-54-2 **MP** (°C)**:** 174
MW: 324.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	2.336E-01	15	K059	2 2 2 0 1	
1.110E-04	3.600E-02	22	M459	0 0 0 0 0	
4.315E-04	1.400E-01	25	F300	1 0 0 0 1	
1.540E-03	4.998E-01	c	D004	0 0 0 0 0	
3.848E-03	1.248E+00	h	D004	0 0 0 0 0	
1.549E-03	5.025E-01	ns	R427	0 0 0 0 0	

4123. $C_{20}H_{24}N_2O_2.3H_2O$
Quinine (trihydrate)
Quinine, compd. with valeric acid (1:1), hydrate
Cinchonan-9-ol, 6′-methoxy-, trihydrate, (8α,9*R*)-
RN: 6151-51-5 **MP** (°C)**:** 57
MW: 378.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-03	6.406E-01	c	D004	0 0 0 0 0	
3.299E-03	1.248E+00	h	D004	0 0 0 0 0	

4124. $C_{20}H_{24}N_2O_4$
Pheniramine maleate
1-Phenyl-1-(2-pyridyl)-3-dimethylaminopropane maleate
Prophenpyridamine maleate
RN: 132-20-7 **MP** (°C)**:**
MW: 356.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	1.105E+01	37.5	L034	2 2 0 1 2	pH 7.4

4125. $C_{20}H_{24}N_2O_5$
Naproxen, *N*-methyl-*N*-carbamoyl methyl-glycolamide ester
RN: **MP** (°C)**:** 179.5
MW: 372.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E-04	5.900E-02	21	B331	1 2 2 1 1	pH 7.4

4126. $C_{20}H_{24}O_3$
Methylsecodione
RN: 80702-24-5 **MP** (°C)**:**
MW: 312.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-03	5.996E-01	25	P324	0 0 0 0 0	

4127. $C_{20}H_{24}O_4$

3,11-Dioxo-4,17(20)-*cis*-pregnadien-21-oic acid methyl ester
U-2726
RN: **MP** (°C)**:**
MW: 328.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	4.300E-03	ns	K029	0 0 2 1 1	

4128. $C_{20}H_{24}O_6$

Dibenzo-18-crown-6
DBC
RN: 14187-32-7 **MP** (°C)**:**
MW: 360.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.025E-05	7.300E-03	25	M127	1 2 1 1 1	
9.000E-05	3.244E-02	26	P029	0 0 0 0 0	

4129. $C_{20}H_{25}ClN_2O_2$

Quinine hydrochloride
Inchonan-9-ol, 6′-methoxy-, monohydrochloride, (8α,9*R*)-
RN: 130-89-2 **MP** (°C)**:**
MW: 360.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	5.497E-01	25	A412	1 0 2 2 1	int

4130. $C_{20}H_{25}ClO_2$

1-Chloro-1,1-dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-24-8 **MP** (°C)**:**
MW: 332.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.708E-07	1.900E-04	rt	C122	0 0 0 0 0	

4131. $C_{20}H_{25}NO_2$

Adiphenine
2-Diethylaminoethyl diphenylacetate
Tranzetil
Patrovine
SKF 962A

RN: 64-95-9 **MP** (°C)**:** 113.5
MW: 311.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	3.114E+00	30	L068	1 0 0 1 0	EFG

4132. $C_{20}H_{25}NO_4$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(diethylamino)-2-oxoethyl ester, (*S*)
Naproxen, *N*,*N*-diethyl glycolamide ester
2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(diethylamino)-2-oxoethyl ester
Naproxen *N*,*N*-diethyl glycolamide ester

RN: 106231-74-7 **MP** (°C)**:** 89
MW: 343.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-05	1.200E-02	21	B331	1 2 2 1 1	pH 7.4
3.494E-05	1.200E-02	21	B331	0 0 0 0 0	

4133. $C_{20}H_{25}NO_4$

3,11-Dioxo-4,17(20)-*cis*-pregnadien-20-oic acid methyl ester 3-oxime

RN: **MP** (°C)**:**
MW: 343.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-05	5.300E-03	ns	K029	0 0 2 1 1	

4134. $C_{20}H_{25}NO_5$

Naproxen, *N*-methyl-*N*-hydroxyethyl glycolamide ester

RN: **MP** (°C)**:** 110
MW: 359.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-04	1.400E-01	21	B331	1 2 2 1 1	pH 7.4

4135. $C_{20}H_{25}NO_6$

2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-[bis(2-hydroxyethyl)amino]-2-oxoethyl ester
Naproxen *N*,*N*-diethanol glycolamide ester
Naproxen,*N*,*N*-dihydroxyethyl glycolamide ester
RN: 114665-20-2 **MP** (°C)**:** 113
MW: 375.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-03	4.100E-01	21	B331	1 2 2 1 1	pH 7.4
1.092E-03	4.100E-01	21	B331	0 0 0 0 0	

4136. $C_{20}H_{26}N_2$

1-(Diphenylmethyl)-4-propylpiperazine
RN: **MP** (°C)**:**
MW: 294.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.448E-04	1.899E-01	25	M438	0 0 0 0 0	

4137. $C_{20}H_{26}N_2O_2$

Ajmaline
Rauwolfine
Ajmalan-17,21-diol, (17R,21α)-
Merabitol
Raugalline
RN: 4360-12-7 **MP** (°C)**:** 159
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	3.591E-01	0	M106	2 1 1 1 0	EFG
1.300E-03	4.244E-01	15	M106	2 1 1 1 0	EFG
1.500E-03	4.897E-01	30	M106	2 1 1 1 0	EFG

4138. $C_{20}H_{26}N_2O_2$

Hydroquinine
Cinchonan-9-ol, 10,11-dihydro-6′-methoxy-, (8α,9*R*)-
10,11-Dihydroquinine
RN: 522-66-7 **MP** (°C)**:** 173.5
MW: 326.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.063E-04	9.999E-02	20	K059	2 2 2 0 1	
>1.53E-03	>5.00E-01	ns	B404	0 2 1 1 0	

4139. $C_{20}H_{26}O_2$
Norethindrone
Norethisterone
RN: 68-22-4 **MP** (°C)**:** 203
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-05	3.981E-03	10	L078	1 0 1 2 0	EFG
1.679E-05	5.012E-03	20	L078	1 0 1 2 0	EFG
2.360E-05	7.043E-03	25	H099	1 0 2 2 2	
1.884E-05	5.623E-03	25	L078	1 0 1 2 2	
8.377E-03	2.500E+00	25	P312	0 0 0 0 0	
2.114E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
3.610E-05	1.077E-02	37	C004	0 0 0 0 0	EFG
2.986E-05	8.912E-03	40	L078	1 0 1 2 0	EFG
4.218E-05	1.259E-02	50	L078	1 0 1 2 0	EFG
3.351E-05	1.000E-02	ns	K444	0 0 0 0 0	

4140. $C_{20}H_{26}O_2$
1,1-Dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 56265-21-5 **MP** (°C)**:**
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-07	4.300E-05	rt	C122	0 0 0 0 0	

4141. $C_{20}H_{26}O_4$
Dicyclohexyl phthalate
1,2-Benzenedicarboxylic acid, dicyclohexyl ester
RN: 84-61-7 **MP** (°C)**:** 66
MW: 330.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E-05	4.000E-03	24	H116	2 1 0 0 2	

4142. $C_{20}H_{27}NO_5S_2$
2-(Acetyloxy)-4-[2-({5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-amino)ehtyl]phenyl acetate
RN: **MP** (°C)**:**
MW: 425.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.151E-04	4.900E-02	ns	S453	0 0 0 0 0	

4143. $C_{20}H_{27}NO_{11}$
Amygdalin
(*R*)-Amygdalin
(*R*)-Laenitrile
(*R*)-Amygdaloside
RN: 29883-15-6 **MP** (°C)**:** 223
MW: 457.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	7.800E+01	10	F300	1 0 0 0 1	
1.698E-01	7.768E+01	ns	R427	0 0 0 0 0	

4144. $C_{20}H_{27}NO_{11}.3H_2O$
Amygdalin (trihydrate)
D-(–)-Amygdalin
(*R*)-Amygdalin
RN: 29883-15-6 **MP** (°C)**:** 214–216
MW: 511.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.504E-01	7.692E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

4145. $C_{20}H_{27}O_4P$
Octyldiphenyl phosphate
Disflamoll DPO
RN: 115-88-8 **MP** (°C)**:**
MW: 362.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.863E-07	1.400E-04	24	H116	2 1 0 0 2	

4146. $C_{20}H_{28}O$
Vitamin A aldehyde
Retinal
All-*trans*-retinal
All-*trans* vitamin A aldehyde
Retinene
RN: 116-31-4 **MP** (°C)**:** 63
MW: 284.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.46E-04	<7.00E-02	25	P312	0 0 0 0 0	

4147. $C_{20}H_{28}O_2$
19-Norprogesterone
19-Norpregn-4-ene-3,20-dione
RN: 472-54-8 **MP** (°C)**:**
MW: 300.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.610E-02	37	L010	2 0 2 1 1	

4148. $C_{20}H_{28}O_2$
Retinoic acid
All-*trans* retinoic acid
3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraenoic acid
β-All-*trans*-retinoic acid
RN: 302-79-4 **MP** (°C)**:** 180-181
MW: 300.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.33E-04	<7.00E-02	25	P312	0 0 0 0 0	

4149. $C_{20}H_{28}O_3$
5,6-Dehydroisoandrosterone formate
Androst-5-en-17-one, 3α-hydroxy-, formate
RN: 4589-84-8 **MP** (°C)**:**
MW: 316.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.424E-05	1.400E-02	ns	B057	0 2 1 1 2	

4150. $C_{20}H_{28}O_3$
Testosterone formate
Androst-4-en-17β-ol-3-one formate
Testosterone 17-formate
RN: 3129-42-8 **MP** (°C)**:**
MW: 316.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-05	4.395E-03	25	J004	1 0 1 1 2	
1.390E-05	4.400E-03	ns	B057	0 2 1 1 1	

4151. $C_{20}H_{29}N_3O_2$
Dibucaine
Cinchocaine
RN: 85-79-0 **MP** (°C)**:** 64
MW: 343.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-04	6.801E-02	ns	B018	0 0 0 0 2	
1.980E-04	6.801E-02	ns	M066	0 0 0 0 2	

4152. $C_{20}H_{30}N_4O_6$
2′-Nonyl-6-methoxypurine arabinoside
4-Quinolinecarboxamide, 2-butoxy-*N*-[2-(diethylamino)ethyl]-
RN: 145913-42-4 **MP** (°C)**:** 88-90
MW: 422.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-04	4.352E-02	37	C348	0 0 0 0 0	pH 7.00

4153. $C_{20}H_{30}O$
D 263
4,6-Diisopropyl-1,1-dimethyl-7-propionylindan
RN: 290294-31-4 **MP** (°C)**:** 117
MW: 286.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.491E-06	1.000E-03	ns	M061	0 0 0 0 0	

4154. $C_{20}H_{30}O$
Vitamin A
Retinol
Afaxin
α-Sterol
RN: 68-26-8 **MP** (°C)**:** 62
MW: 286.46 **BP** (°C)**:** 137–138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.49E-05	<1.00E-02	25	P312	0 0 0 0 0	

4155. $C_{20}H_{30}O_2$
Abietic acid
13-Isopropylpodocarpa-7,13-dien-15-oic acid
Sylvic acid
RN: 514-10-3 **MP** (°C)**:** 172
MW: 302.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	4.839E-02	20	B009	2 2 1 2 0	

4156. $C_{20}H_{30}O_2$
17-Methyltestosterone
17-α-Methyltestosterone
Methyltestosterone
Methyl-testosterone
RN: 58-18-4 **MP** (°C)**:** 161
MW: 302.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-04	3.720E-02	20	F012	1 0 1 1 1	
1.120E-04	3.388E-02	25	H099	1 0 2 2 2	
1.058E-04	3.200E-02	25	K003	2 1 1 1 1	
4.400E-02	1.331E+01	25	M379	1 0 1 1 0	EFG,*sic*
<5.62E-04	<1.70E-01	25	P312	0 0 0 0 0	
2.313E-03	6.995E-01	25	P324	0 0 0 0 0	
1.018E-04	3.080E-02	30	T005	2 0 2 2 2	
1.200E-04	3.630E-02	37	E014	2 2 2 1 2	pH 7.3
7.472E-05	2.260E-02	ns	B057	0 2 1 1 2	
9.918E-05	3.000E-02	rt	N302	0 2 1 2 1	

4157. $C_{20}H_{30}O_3$
Androstanolone formate
5α-Androstan-3-one, 17-hydroxy-, formate
RN: 4589-90-6 **MP** (°C)**:**
MW: 318.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-06	1.490E-03	ns	B057	0 2 1 1 2	

4158. $C_{20}H_{30}O_6$
Butyl glycol phthalate
bis(2-Butoxyethyl) phthalate
Dibutoxyethyl phthalate
bis(2-*N*-Butoxyethyl) phthalate
RN: 117-83-9 **MP** (°C)**:** 230
MW: 366.46 **BP** (°C)**:** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.458E-05	2.000E-02	15	H069	1 0 1 1 0	
<8.18E-04	<3.00E-01	20	F070	1 0 0 0 1	

4159. $C_{20}H_{31}NO$
Trihexyphenidyl
1-Phenyl-1-cyclohexyl-3-piperidyl-1-propanol hydrochloride
Artane
Benzhexol chloride
Trihexyphenidyl-D,L hydrochloride
Tremin
RN: 52-49-3 **MP** (°C)**:**
MW: 301.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	6.709E-04	22.5	B440	0 0 0 0 0	

4160. $C_{20}H_{31}NO_3$
Acetaminophen laurate
Acetaminophen dodecanoate
RN: 54942-38-0 **MP** (°C)**:** 111
MW: 333.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E-05	6.000E-03	25	B010	1 1 1 1 0	

4161. $C_{20}H_{32}O_3$
Tridecyl *p*-hydroxybenzoate
p-Hydroxybenzoic acid tridecyl ester
RN: 69679-32-9 **MP** (°C)**:**
MW: 320.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	3.639E-01	25	D081	1 2 2 1 2	

4162. $C_{20}H_{32}O_5$
Dinoprostone
Prostaglandin E2
RN: 363-24-6 **MP** (°C)**:** 66–68
MW: 352.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.123E-03	1.101E+00	8.53	F068	0 0 2 2 0	
4.022E-03	1.418E+00	19.24	F068	0 0 2 2 0	
4.173E-03	1.471E+00	25.35	F068	0 0 2 2 0	
4.575E-03	1.613E+00	29.9	F068	0 0 2 2 0	

4163. $C_{20}H_{33}NO$
Fenpropimorph
4-(3-(4-(1,1-Dimethylethyl)phenyl)-2-methylpropyl)-2,6-dimethylmorpholine
Corbe
Mistral
RN: 67306-03-0 **MP** (°C)**:**
MW: 303.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-05	4.300E-03	ns	V414	0 0 0 0 0	

4164. $C_{20}H_{33}NO_3$
4-Heptoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-75-0 **MP** (°C)**:**
MW: 335.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.677E-02	ns	M066	0 0 0 0 1	

4165. $C_{20}H_{33}N_3O_4$
Celiprolol
RN: 56980-93-9 **MP** (°C)**:**
MW: 379.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	2.290E-02	22.5	B440	0 0 0 0 0	
6.008E-09	2.280E-06	200	M418	0 0 0 0 0	

4166. $C_{20}H_{34}$
5-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4167. $C_{20}H_{34}$
2-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4168. $C_{20}H_{34}$
4-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4169. $C_{20}H_{34}$
3-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4170. $C_{20}H_{34}$
6-Phenyltetradecane
RN: **MP** (°C)**:**
MW: 274.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4171. $C_{20}H_{34}N_2O_2$

4-Heptylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: **MP** (°C)**:**

MW: 334.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	7.025E-02	ns	M066	0 0 0 0 1	

4172. $C_{20}H_{34}O_4$

4-Octylphenol triethoxylate

RN: 51437-91-3 **MP** (°C)**:**

MW: 338.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.436E-05	1.840E-02	20.5	A335	0 0 0 0 0	
5.440E-05	1.841E-02	20.5	A335	0 0 0 0 0	

4173. $C_{20}H_{34}O_8$

Acetyl tributyl citrate

1,2,3-Propanetricarboxylic acid

Tributyl acetylcitrate

RN: 77-90-7 **MP** (°C)**:**

MW: 402.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.224E-06	1.700E-03	25	F067	1 0 2 2 1	

4174. $C_{20}H_{36}O_4$

Dioctyl maleate

2-Butenedioic acid (Z)-

Dioctyl ester

RN: 2915-53-9 **MP** (°C)**:**

MW: 340.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E-06	6.000E-04	25	F067	1 0 2 2 2	

4175. $C_{20}H_{36}O_6$
Dicyclohexyl-18-crown-6
Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, icosahydro-
Dicyclohexano-18-crown-6
cis-Dicyclohexano-18-crown-6
RN: 16069-36-6 **MP** (°C)**:**
MW: 372.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-02	1.341E+01	26	P029	0 0 0 0 0	
2.200E-02	8.195E+00	53	P029	0 0 0 0 0	
1.000E-02	3.725E+00	82	P029	0 0 0 0 0	

4176. $C_{20}H_{40}$
1-Eicosene
n-Eicosene
RN: 3452-07-1 **MP** (°C)**:**
MW: 280.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-12	5.350E-10	23	C332	0 0 0 0 0	

4177. $C_{21}H_{11}ClF_6N_2O_3$
Flufenoxuron
RN: 101463-69-8 **MP** (°C)**:**
MW: 488.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-09	3.800E-06	20	M402	0 0 0 0 0	

4178. $C_{21}H_{13}N$
1:2,6:7-Dibenzacridine
RN: 226-92-6 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.397E-05	22	B175	1 0 1 1 0	

4179. $C_{21}H_{13}N$
1:2,8:9-Dibenzacridine
RN: 224-53-3 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-08	1.955E-05	22	B175	1 0 1 1 0	

4180. $C_{21}H_{13}N$
3:4,6:7-Dibenzacridine
RN: 226-97-1 **MP** (°C)**:**
MW: 279.34 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	6.984E-05	22	B175	1 0 1 1 1	

4181. $C_{21}H_{14}$
5-Methyl-3,4-benzpyrene
RN: 31647-36-6 **MP** (°C)**:** 216
MW: 266.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-09	8.000E-07	27	D003	1 0 0 1 0	

4182. $C_{21}H_{15}ClN_2O_4S$
1-(*p*-Chlorobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-38-4 **MP** (°C)**:**
MW: 426.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.965E-07	3.400E-04	37	F183	1 0 1 1 2	intrinsic

4183. $C_{21}H_{15}N_3O_6S$
1-(*p*-Nitrobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 21413-53-6 **MP** (°C)**:**
MW: 437.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.486E-06	6.500E-04	37	F183	1 0 1 1 2	intrinsic

4184. $C_{21}H_{16}$
3-Methylcholanthrene
1,2-Dihydro-3-methyl-benz[j]aceanthrylene
20-Methylcholanthrene
RN: 56-49-5 **MP** (°C)**:** 179
MW: 268.36 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E-08	3.230E-06	24	H106	1 0 2 2 2	
1.081E-08	2.900E-06	25	M064	1 1 2 2 1	
1.204E-08	3.230E-06	25	M156	1 2 1 1 2	
1.100E-08	2.952E-06	25	M342	1 0 1 1 1	
5.589E-09	1.500E-06	27	D003	1 0 0 1 1	
1.081E-08	2.900E-06	ns	M344	0 0 0 0 1	

4185. $C_{21}H_{16}N_2O_2$
C.I. Disperse blue 24
9,10-Anthracenedione, 1-amino-4-hydroxy-2-phenoxy-
Serilene red 2BL
Sumikaron red E-FBL
Solvent red 146
RN: 17418-58-5 **MP** (°C)**:** 151
MW: 328.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.642E-05	25	B333	0 0 0 0 0	

4186. $C_{21}H_{16}N_2O_4S$
1-Benzenesulfonyl-5,5-diphenyl-hydantoin
RN: 21413-28-5 **MP** (°C)**:**
MW: 392.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.587E-06	1.800E-03	37	F183	1 0 1 1 2	intrinsic

4187. $C_{21}H_{16}N_2O_5S$
1-(*p*-Hydroxylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-35-1 **MP** (°C)**:**
MW: 408.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.080E-06	3.300E-03	37	F183	1 0 1 1 2	intrinsic

4188. $C_{21}H_{17}N_3O_2S_2$
2-Sulfanilamido-4-*p*-diphenylthiazole
RN: **MP** (°C)**:**
MW: 407.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-06	1.000E-03	37	R045	1 2 1 1 0	

4189. $C_{21}H_{17}N_3O_4S$
1-(*p*-Aminobenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-34-0 **MP** (°C)**:**
MW: 407.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.436E-06	1.400E-03	37	F183	1 0 1 1 2	intrinsic

4190. $C_{21}H_{19}NO_4$
Cinmetacin
1-Cinnamoyl-2-methyl-5-methoxyindolyl-3-acetic acid
Indolacin
RN: 20168-99-4 **MP** (°C)**:** 170
MW: 349.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.86E-06	<1.00E-03	25	K027	2 0 2 2 0	

4191. $C_{21}H_{20}Cl_2O_3$
Permethrin
3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl Ester
Ambush
Pounce
Ectiban
RN: 52645-53-1 **MP** (°C)**:** 36.5
MW: 391.30 **BP** (°C)**:** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.111E-07	2.000E-04	ns	M161	0 0 0 0 0	
~5.11E-07	~2.00E-04	ns	Y418	0 0 0 0 0	

4192. $C_{21}H_{20}O_9$
Puerarin
8-ß-D-Glucopyransyl-7-hydroxy-3-(4-hydroxyphenyl)-4H-1benzopyran-4-one
RN: 3681-99-0 **MP** (°C)**:**
MW: 416.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-01	3.373E+02	15.0	W418	0 0 0 0 0	
9.500E-01	3.956E+02	20.0	W418	0 0 0 0 0	
1.100E+00	4.580E+02	25.0	W418	0 0 0 0 0	
1.260E+00	5.246E+02	30.0	W418	0 0 0 0 0	
1.420E+00	5.913E+02	35.0	W418	0 0 0 0 0	
1.710E+00	7.120E+02	40.0	W418	0 0 0 0 0	
2.020E+00	8.411E+02	45.0	W418	0 0 0 0 0	
2.430E+00	1.012E+03	50.0	W418	0 0 0 0 0	
2.840E+00	1.183E+03	55.0	W418	0 0 0 0 0	

4193. $C_{21}H_{21}ClN_2O_8$

Demeclocycline
Declomycin
Methylchlorotetracycline
Demethylchlortetracycline

RN: 127-33-3 **MP** (°C)**:**
MW: 464.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-03	1.515E+00	21	M044	2 0 2 2 2	
3.012E-03	1.400E+00	25	B191	1 0 0 0 1	neutral pH

4194. $C_{21}H_{21}N$

Cyproheptadine

RN: 129-03-3 **MP** (°C)**:**
MW: 287.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	3.176E-04	22.5	B440	0 0 0 0 0	

4195. $C_{21}H_{21}NO_6$

Rhoeadine
[1,3]Dioxolo[4,5-h]-1,3-dioxolo[7,8][2]benzopyrano[3,4-a][3]benzazepine, 5β,6,7,8,13β,15-hexahydro-15-methoxy-6-methyl-, (5b*R*,13b*R*,15*S*)
8-Methoxy-16-methyl-2,3:10,11-bis[methylenebis(oxy)]-, (8β)-

RN: 2718-25-4 **MP** (°C)**:** 245–247dec
MW: 383.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.172E-03	8.326E-01	25	D004	0 0 0 0 0	

4196. $C_{21}H_{21}NO_6$

Hydrastine
Hydrastin
(1*R*,9*S*)-β-Hydrastine

RN: 118-08-1 **MP** (°C)**:** 132
MW: 383.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-04	3.144E-01	15	K059	2 2 2 0 1	
7.825E-05	3.000E-02	20	F300	1 0 0 0 1	

4197. $C_{21}H_{21}N_3O_3S$
L-Phe-dapsone
Benzenepropanamide, α-amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-
RN: 160349-01-9 **MP** (°C)**:**
MW: 395.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.057E-06	2.000E-03	25	P351	0 0 0 0 0	pH 7.4
3.287E-03	1.300E+00	25	P351	0 0 0 0 0	

4198. $C_{21}H_{21}O_4P$
Tricresyl phosphate
Tritolyl phosphate
Tri-*p*-cresyl phosphate
RN: 1330-78-5 **MP** (°C)**:**
MW: 368.37 **BP** (°C)**:** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.009E-07	7.400E-05	24	H116	2 1 0 0 1	
2.715E-07	1.000E-04	25	F067	1 0 2 2 1	
2.172E-04	7.999E-02	ns	F014	0 0 0 0 0	

4199. $C_{21}H_{22}N_2O_2$
Strychnine
Strychnidin-10-one
Gopher Getter
L-Strychnine
Gopher Bait
RN: 57-24-9 **MP** (°C)**:** 275
MW: 334.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	9.029E-02	15	K059	2 2 2 0 1	
4.186E-04	1.400E-01	20.0	N002	2 1 2 2 1	
5.980E-04	2.000E-01	30.0	N002	2 1 2 2 1	
1.017E-03	3.400E-01	40.0	N002	2 1 2 2 1	
1.196E-03	4.000E-01	50.0	N002	2 1 2 2 1	
1.346E-03	4.500E-01	60.0	N002	2 1 2 2 1	
1.794E-03	6.000E-01	75.0	N002	2 1 2 2 1	
4.672E-04	1.562E-01	c	D004	0 0 0 0 0	
9.643E-04	3.225E-01	h	D004	0 0 0 0 0	
4.276E-04	1.430E-01	rt	M161	0 0 0 0 2	

4200. $C_{21}H_{22}N_2O_5$

Benzeneacetic acid, 4-benzoyl-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

N-Methyl-*N*-carbamoyl methyl glycolamide salicylate

RN: 114665-16-6 **MP** (°C)**:** 83

MW: 382.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	0 0 0 0 0	

4201. $C_{21}H_{22}N_2O_5$

Ketoprofen, *N*-methyl-*N*-carbamoylmethyl glycolamide ester

Benzeneacetic acid, 3-benzoyl-α-methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

RN: 116482-84-9 **MP** (°C)**:** 83.5

MW: 382.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	1 2 2 1 1	pH 7.4

4202. $C_{21}H_{23}ClFNO_2$

Haloperidol

Haldol

4-[4-(*p*-Chlorophenyl)-4-hydroxypiperidino]-4′-fluorobutyrophenone

Serenace

RN: 52-86-8 **MP** (°C)**:** 148

MW: 375.87 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.623E-04	6.100E-02	22	J420	0 0 0 0 0	pH6.5
5.474E-06	2.058E-03	22.5	B440	0 0 0 0 0	
7.981E-06	3.000E-03	30	P044	0 0 0 0 0	
2.660E-05	1.000E-02	ns	K444	0 0 0 0 0	
<2.66E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4203. $C_{21}H_{23}N_3OS$

Pericyazine

2-Cyano-10-[3′-(4″-hydroxypiperidino)propyl]phenothiazine

Periciazine

RN: 2622-26-6 **MP** (°C)**:** 116

MW: 365.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.801E-02	37	F011	1 0 1 1 2	pH 7.4

4204. $C_{21}H_{24}FN_3O_7$
3-Quinolinecarboxylic acid
7-[4-[[1-(Acetyloxy)ethoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-
RN: 99106-35-1 **MP** (°C)**:** 216
MW: 449.44 **BP** (°C)**:** 636.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.122E-04	4.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.112E-04	5.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
1.112E-05	5.000E-03	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
1.335E-04	6.000E-02	25	A414	1 0 1 1 1	

4205. $C_{21}H_{24}F_3N_3S$
Trifluoperazine
Stelazine
RN: 117-89-5 **MP** (°C)**:** 232
MW: 407.50 **BP** (°C)**:** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.223E-02	24	G022	2 0 1 1 1	
3.600E-05	1.467E-02	37	F011	1 0 1 1 1	pH 7.4

4206. $C_{21}H_{25}NO$
4-Cyano-4′-octyloxybiphenyl
8 COB
RN: **MP** (°C)**:**
MW: 307.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-07	8.301E-05	21	D300	2 2 1 1 2	

4207. $C_{21}H_{25}N_5O_5$
Benzoic acid, 4-(4-morpholinylmethyl)-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-75-5 **MP** (°C)**:**
MW: 427.46 **BP** (°C)**:** 712.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-03	7.700E-01	21	B419	1 1 2 2 1	int

4208. $C_{21}H_{26}ClN_3OS$
Perphenazine
4-(3-(2-Chlorophenothiazin-10-YL)propyl)-1-piperazineethanol
Etrafon
Trilafon
RN: 58-39-9 **MP** (°C)**:** 97
MW: 403.98 **BP** (°C)**:** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	2.828E-02	24	G022	2 0 1 1 1	

4209. $C_{21}H_{26}FN_3O_4$
Permafloxacin
RN: 143383-65-7 **MP** (°C)**:**
MW: 403.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-02	7.477E+00	25	F415	0 0 0 0 0	Average

4210. $C_{21}H_{26}N_2O_3$
1-(2,3-Dihydro-5-methoxybenzo[b]furan-2-ylmethyl)-4-(*o*-methoxyphenyl)piperazine
RN: **MP** (°C)**:**
MW: 354.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.642E-05	2.000E-02	37	L079	1 0 1 1 0	intrinsic

4211. $C_{21}H_{26}N_2S_2$
Thioridazine
10H-Phenothiazine
10-[2-(1-Methyl-2-piperidyl)ethyl]-2-methylthio
Aldazine
Mellaril
Melleril
RN: 50-52-2 **MP** (°C)**:**
MW: 370.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	1.113E-03	22.5	B440	0 0 0 0 0	

4212. $C_{21}H_{26}O_4$
Lifibrol
Benzoic acid, 4-[4-[4-(1,1-dimethylethyl)phenyl]-2-hydroxybutoxy]-
RN: 96609-16-4 **MP** (°C)**:**
MW: 342.44 **BP** (°C)**:** 536.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.301E-04	12.0	B412	1 0 2 2 1	mod 2 crystal
8.600E-07	2.945E-04	12.0	B412	1 0 2 2 1	mod I crystal
7.000E-07	2.397E-04	20.0	B412	1 0 2 2 1	mod 2 crystal
1.110E-06	3.801E-04	20.0	B412	1 0 2 2 1	mod 1 crystal
1.070E-06	3.664E-04	29.0	B412	1 0 2 2 1	mod 2 crystal
1.640E-06	5.616E-04	29.0	B412	1 0 2 2 1	mod 1 crystal
2.090E-06	7.157E-04	38.0	B412	1 0 2 2 1	mod 2 crystal
2.740E-06	9.383E-04	38.0	B412	1 0 2 2 1	mod 1 crystal
3.080E-06	1.055E-03	47.0	B412	1 0 2 2 1	mod 2 crystal
4.890E-06	1.675E-03	47.0	B412	1 0 2 2 1	mod 1 crystal
4.690E-06	1.606E-03	54.0	B412	1 0 2 2 1	mod 2 crystal
5.900E-06	2.020E-03	54.0	B412	1 0 2 2 1	mod 1 crystal

4213. $C_{21}H_{26}O_4$
17-Hydroxy-6-methyl-16-methylenepregna-4,6-diene-3,20-dione acetate
RN: **MP** (°C)**:**
MW: 342.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-06	2.900E-03	37	H004	0 0 0 0 0	

4214. $C_{21}H_{26}O_5$
Prednisone
1,4-Pregnadiene-17α,21-diol-3,11,20-trione
1,4-Pregnadiene-17x,21-diol-3,11,20-trione
Delcortin
Metocorten
Panasol
RN: 53-03-2 **MP** (°C)**:** 234
MW: 358.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-04	1.150E-01	25	K003	2 1 1 1 1	
2.734E-04	9.799E-02	ns	B404	0 2 1 1 0	

4215. $C_{21}H_{27}FO_5$

Fluprednisolone
6α-Fluoro-11β,17,21-trihydroxypregna-1,4-diene-3,20-dione17,21-trihydroxypregna-1,4-diene-3,20-dione
Alphadrol
RN: 53-34-9 **MP** (°C)**:**
MW: 378.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-03	1.040E+00	37	H004	0 0 0 0 0	

4216. $C_{21}H_{27}FO_5.H_2O$

Fluprednisolone (monohydrate)
RN: 53-34-9 **MP** (°C)**:**
MW: 396.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	5.860E-01	37	H004	0 0 0 0 0	

4217. $C_{21}H_{27}FO_6$

Triamcinolone
9α-Fluoro-11β,16α,17α,21-tetrahydroxy-1,4-pregnadiene-3,20-dione
9α-Fluoro-16α-hydroxyprednisolone
Aristocort
RN: 124-94-7 **MP** (°C)**:** 269
MW: 394.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-04	7.999E-02	25	F024	1 0 0 0 0	
4.260E-04	1.680E-01	37	C400	2 0 2 2 2	

4218. $C_{21}H_{27}NO_3$

Propafenone
RN: 54063-53-5 **MP** (°C)**:**
MW: 341.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	7.599E-04	22.5	B440	0 0 0 0 0	

4219. $C_{21}H_{28}N_2$
1-(Diphenylmethyl)-4-butylpiperazine
RN: **MP** (°C)**:**
MW: 308.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	4.816E-01	25	M438	0 0 0 0 0	

4220. $C_{21}H_{28}N_4O_7$
Pentyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 448.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	2.646E-01	25	M316	1 1 1 1 2	

4221. $C_{21}H_{28}O_2$
Norgestrel
Microlut
Microval
RN: 797-63-7 **MP** (°C)**:** 206
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4222. $C_{21}H_{28}O_2$
Ethisterone
17α-Ethynyl testosterone
Ethynyl testosterone
Gestoral
Pregneninolone
Anhydrohydroxyprogesterone
RN: 434-03-7 **MP** (°C)**:** 269
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-06	5.999E-04	20	G072	1 2 2 1 2	
1.600E-06	4.999E-04	20	L077	1 2 2 2 1	
1.280E-06	4.000E-04	25	K003	2 1 1 1 1	
2.200E-06	6.874E-04	27.34	L077	1 2 2 2 1	
3.200E-06	9.999E-04	35	L077	1 2 2 2 1	
3.500E-06	1.094E-03	42.34	L077	1 2 2 2 1	
4.200E-06	1.312E-03	50	L077	1 2 2 2 1	

4223. $C_{21}H_{28}O_2$
1,1,1-Trimethyl-2,2-bis(*p*-ethoxylphenyl)ethane
RN: 27955-87-9 **MP** (°C)**:**
MW: 312.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-07	1.400E-04	rt	C122	0 0 0 0 0	

4224. $C_{21}H_{28}O_5$
Prednisolone
11β,17α,21-Trihydroxypregna-1,4-diene-3,20-dione
Ropredlone
Predonin
Hostacortin H
Nisolone
RN: 50-24-8 **MP** (°C)**:** 240
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.173E-03	2.225E+00	25	G008	1 2 1 1 2	*sic*
5.963E-04	2.150E-01	25	K003	2 1 1 1 1	
1.379E-03	4.970E-01	25	K021	1 2 2 2 1	
5.770E-04	2.080E-01	25	M457	0 0 0 0 0	
7.000E-04	2.523E-01	30	H016	2 2 2 2 0	EFG
1.268E-03	4.570E-01	30	T002	1 0 2 0 2	anhydrous, form A
1.398E-03	5.040E-01	30	T002	1 0 2 0 2	anhydrous, form B
6.658E-04	2.400E-01	30	T002	1 0 2 0 2	hydrate
6.658E-04	2.400E-01	30	W006	2 2 2 1 2	hydrate, form C
4.694E-04	1.692E-01	37	C400	2 0 2 2 2	
9.738E-04	3.510E-01	37	H004	0 0 0 0 0	
5.500E-04	1.982E-01	ns	F327	0 0 1 2 2	
2.774E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.398E-03	5.040E-01	ns	W006	2 2 2 1 2	anhydrous, form B

4225. $C_{21}H_{28}O_5$
Aldosterone
18-Oxocorticosterone
Aldocortin
Electrocortin
18-Oxo-11β,21-dihydroxy-4-pregnene-3,20-dione
RN: 52-39-1 **MP** (°C)**:** 108
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	5.118E-02	37	H034	1 0 2 1 2	pH 7.4
1.413E-04	5.092E-02	ns	R427	0 0 0 0 0	

4226. $C_{21}H_{28}O_5$
Cortisone
17-Hydroxy-11-dehydrocorticosterone
Cortate
RN: 53-06-5 **MP** (°C)**:** 222
MW: 360.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.766E-04	2.799E-01	20	D041	1 0 0 0 0	
6.379E-04	2.299E-01	25	K003	2 1 1 1 1	
7.768E-04	2.800E-01	25	M023	1 0 2 1 1	
7.500E-04	2.703E-01	30	L344	2 0 1 1 0	EFG
6.000E-04	2.163E-01	37	E014	2 2 2 1 2	pH 7.3
7.768E-04	2.800E-01	ns	B338	0 0 0 0 1	

4227. $C_{21}H_{29}FO_5$
Fludrocortisone
9α-Fluoro-17-hydroxycorticosterone
9α-Fluorohydrocortisone
Florinef
RN: 127-31-1 **MP** (°C)**:** 260dec
MW: 380.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E-04	1.110E-01	25	K021	1 2 2 2 1	
8.516E-04	3.240E-01	25	L009	1 0 0 1 1	
2.411E-04	9.172E-02	37	C400	2 0 2 2 2	

4228. $C_{21}H_{29}NO$
N,*N*-Dicyclohexylcinnamamide
N,*N*-Dicyclohexyl-3-phenyl2-propenamide
RN: 6631-21-6 **MP** (°C)**:**
MW: 311.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.680E-06	1.769E-03	ns	H350	0 0 0 0 0	

4229. $C_{21}H_{29}N_3O$
Disopyramide
α-(2-(Diisopropylamino)ethyl)-α-phenyl-2-pyridineacetamide
RN: 3737-09-5 **MP** (°C)**:**
MW: 339.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.817E-05	6.170E-03	22.5	B440	0 0 0 0 0	
1.995E-02	6.774E+00	ns	R427	0 0 0 0 0	

4230. $C_{21}H_{30}N_4O_{10}$
Methylol riboflavine
Methylol-riboflavin
RN: **MP** (°C)**:**
MW: 498.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-02	1.190E+01	20	F300	1 0 0 0 2	compound not stable

4231. $C_{21}H_{30}N_6O_4S$
Benzenesulfonamide, *N*-[2-(dimethylamino)ethyl]-4-(2,3,4,5,6,7-hexahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-
RN: 89073-58-5 **MP** (°C)**:** 270dec
MW: 462.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	1.990E+01	ns	H316	0 0 0 0 0	0.1N HCL
1.081E-04	5.000E-02	ns	H316	0 0 0 0 0	pH 7.4

4232. $C_{21}H_{30}O_2$
Tetrahydrocannabinol
THC
Dronabinol
δ9-Tetrahydrocannabinol
RN: 1972-08-3 **MP** (°C)**:**
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.904E-06	2.800E-03	23	G018	1 0 0 1 0	

4233. $C_{21}H_{30}O_2$
Progesterone
δ4-Pregnene-3,20-dione
Corlutin
Corlutina
Lutein
Pregn-4-ene-3,20-dione
RN: 57-83-0 **MP** (°C)**:** 121
MW: 314.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-05	5.346E-03	10	B012	2 0 1 1 0	
2.200E-05	6.918E-03	20	B012	2 0 1 1 0	
3.210E-05	1.009E-02	20	L077	1 2 2 2 2	
2.600E-05	8.176E-03	21.70	M108	1 2 1 1 2	form A

(*continued*)

4233. $C_{21}H_{30}O_2$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.837E-05	1.521E-02	23	B014	0 0 1 2 2	
3.720E-05	1.170E-02	24.00	M108	1 2 1 1 2	form B
2.800E-05	8.805E-03	25	B012	2 0 1 1 0	
2.512E-05	7.899E-03	25	B041	1 0 2 2 0	EFG
3.802E-05	1.196E-02	25	F312	1 1 2 2 2	units assumed
2.862E-05	9.000E-03	25	K003	2 1 1 1 1	
6.359E-04	2.000E-01	25	P324	0 0 0 0 0	
2.810E-05	8.837E-03	25.30	M108	1 2 1 1 2	form A
3.690E-05	1.160E-02	27.34	L077	1 2 2 2 2	
3.600E-05	1.132E-02	30	B012	2 0 1 1 0	
3.498E-05	1.100E-02	30	M007	2 2 1 2 2	average of 8
3.800E-05	1.195E-02	30.20	M108	1 2 1 1 2	form A
4.520E-05	1.421E-02	30.50	M108	1 2 1 1 2	form B
4.230E-05	1.330E-02	35	L077	1 2 2 2 2	
5.390E-05	1.695E-02	35.50	M108	1 2 1 1 2	form B
4.690E-05	1.475E-02	36.40	M108	1 2 1 1 2	form A
3.816E-05	1.200E-02	37	A086	1 0 1 1 2	
3.528E-05	1.109E-02	37	C400	2 0 2 2 2	
4.800E-05	1.509E-02	37	H034	1 0 2 1 2	pH 7.4
4.260E-05	1.340E-02	37	H035	1 1 1 1 2	pH 7.4
4.007E-05	1.260E-02	37	L010	2 0 2 1 1	
4.260E-05	1.340E-02	37.50	B041	1 0 2 2 2	
3.981E-05	1.252E-02	37.50	B041	1 0 2 2 0	EFG
3.800E-05	1.195E-02	40	B012	2 0 1 1 0	
6.750E-05	2.123E-02	40.70	M108	1 2 1 1 2	form B
6.370E-05	2.003E-02	41.30	M108	1 2 1 1 2	form A
4.580E-05	1.440E-02	42.34	L077	1 2 2 2 2	
6.500E-05	2.044E-02	46.10	M108	1 2 1 1 2	form A
4.900E-05	1.541E-02	50	B012	2 0 1 1 0	
4.930E-05	1.550E-02	50	L077	1 2 2 2 2	
		amb	L434	0 0 0 0 0	
1.908E-05	6.000E-03	ns	B404	0 2 1 1 0	

4234. $C_{21}H_{30}O_3$

Deoxycorticosterone
21-Hydroxyprogesterone
4-Pregnen-21-ol-3,20-dione
11-Deoxycorticosterone
21-Hydroxypregn-4-ene-3,20-dione

RN: 64-85-7 **MP** (°C)**:** 141.5
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.387E-04	1.450E-01	25	K003	2 1 1 1 1	
4.588E-04	1.516E-01	37	C400	2 0 2 2 2	
1.800E-04	5.948E-02	37	E014	2 2 2 1 2	pH 7.3
1.070E-04	3.536E-02	37	H034	1 0 2 1 2	pH 7.4

4235. $C_{21}H_{30}O_3$
11α-Hydroxyprogesterone
11α-Hydroxy-4-pregnene-3,20-dione
RN: 80-75-1 **MP** (°C)**:**
MW: 330.47 **BP** (°C)**:** 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E-04	1.164E-01	37	C400	2 0 2 2 2	

4236. $C_{21}H_{30}O_3$
11β-Hydroxyprogesterone
11β-Hydroxypregn-4-ene-3,20-dione
RN: 600-57-7 **MP** (°C)**:**
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	3.084E-02	37	C400	2 0 2 2 2	

4237. $C_{21}H_{30}O_3$
5,6-Dehydroisoandrosterone acetate
Androst-5-en-17-one, 3-(acetyloxy)-, (3β)-
RN: 853-23-6 **MP** (°C)**:** 166
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-05	1.150E-02	ns	B057	0 2 1 1 2	

4238. $C_{21}H_{30}O_3$
Testosterone acetate
17-*O*-Acetyltestosterone
Androst-4-en-3-one, 17-(acetyloxy)-, (17β)-
RN: 1045-69-8 **MP** (°C)**:** 140
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.111E-06	2.350E-03	25	J004	1 0 1 1 2	
7.111E-06	2.350E-03	ns	B057	0 2 1 1 2	

4239. $C_{21}H_{30}O_3$
17-α-Hydroxyprogesterone
Pregn-4-ene-3,20-dione, 17-hydroxy-
Prodix
Prodox
U 3096
RN: 68-96-2 **MP** (°C)**:** 222
MW: 330.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-05	5.056E-03	20	L077	1 2 2 2 2	
1.960E-05	6.477E-03	27.34	L077	1 2 2 2 2	
2.760E-05	9.121E-03	35	L077	1 2 2 2 2	
3.580E-05	1.183E-02	42.34	L077	1 2 2 2 2	
4.290E-05	1.418E-02	50	L077	1 2 2 2 2	

4240. $C_{21}H_{30}O_4$
Corticosterone
11,21-Dihydroxyprogesterone
δ(4)-Pregnene-11β,21-diol-3,20-dione
11β,21-Dihydroxypregn-4-ene-3,20-dione
RN: 50-22-6 **MP** (°C)**:** 182
MW: 346.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.943E-04	2.405E-01	37	C400	2 0 2 2 2	

4241. $C_{21}H_{30}O_4$
11β,17α-Dihydroxy-4-pregnene-3,20-dione
Pregn-5-ene-3,20-dione, 11,17-dihydroxy-
Pregn-5-ene-3,20-dione, 11b,17-dihydroxy-
RN: 603-97-4 **MP** (°C)**:**
MW: 346.47 **BP** (°C)**:** 516.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.361E-04	8.180E-02	37	C400	2 0 2 2 2	

4242. $C_{21}H_{30}O_4$
Cortexolone
11-Deoxy-17-hydroxycorticosterone
11-Deoxycortisol
11-Desoxycortisone
17,21-Dihydroxy-4-pregnene-3,20-dione
17α,21-Dihydroxypregn-4-ene-3,20-dione
RN: 152-58-9 **MP** (°C)**:** 208
MW: 346.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-04	4.408E-02	37	C400	2 0 2 2 2	

4243. $C_{21}H_{30}O_5$
Hydrocortisone
11β,17,21-Trihydroxypregn-4-ene-3,20-dione
Colifoam
Cortaid
Cortef
Bactine
RN: 50-23-7 **MP** (°C)**:** 218.5
MW: 362.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.733E-01	10	B012	2 0 1 1 0	
7.725E-04	2.800E-01	20	A067	0 0 0 0 1	
7.430E-04	2.693E-01	20	B012	2 0 1 1 0	
8.109E-04	2.939E-01	22.5	B422	2 0 2 2 2	
8.820E-04	3.197E-01	25	B012	2 0 1 1 0	
9.932E-04	3.600E-01	25	C437	0 0 0 0 0	Average
7.725E-04	2.800E-01	25	H015	1 0 0 0 1	
8.194E-04	2.970E-01	25	H098	1 0 2 0 2	
8.190E-04	2.969E-01	25	H320	0 0 0 0 0	
8.194E-04	2.970E-01	25	H320	0 0 0 0 0	
7.860E-04	2.849E-01	25	K003	2 1 1 1 1	
1.614E-03	5.850E-01	25	K021	1 2 2 2 1	
7.725E-04	2.800E-01	25	M023	1 0 2 1 1	
9.896E-03	3.587E+00	25	P324	0 0 0 0 0	
1.034E-03	3.748E-01	30	B012	2 0 1 1 0	
1.000E-03	3.625E-01	30	L344	2 0 1 1 0	EFG
1.077E-03	3.905E-01	37	C400	2 0 2 2 2	
1.070E-03	3.878E-01	37	H036	1 0 2 2 2	EFG
1.265E-03	4.585E-01	40	B012	2 0 1 1 0	
1.519E-03	5.506E-01	50	B012	2 0 1 1 0	
7.725E-04	2.800E-01	298	F016	0 0 0 0 0	
1.159E-03	4.200E-01	amb	L434	0 0 0 0 0	
1.104E-03	4.000E-01	amb	L445	0 0 0 0 0	Intrinsic
7.116E-04	2.579E-01	ns	B404	0 2 1 1 0	

4244. $C_{21}H_{30}O_6$
Cortisone acetate
Pregn-4-ene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-
RN: 50-04-4 **MP** (°C)**:** 235
MW: 378.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.284E-05	2.000E-02	22.5	G301	0 0 0 0 0	
5.020E-05	1.900E-02	25	K003	2 1 1 1 1	
5.284E-05	2.000E-02	25	M023	1 0 2 1 0	
7.398E-05	2.800E-02	25	P096	0 0 0 0 0	
1.000E-04	3.785E-02	30	L068	1 0 0 1 0	EFG

4245. $C_{21}H_{31}NO$
N-Cyclododecylcinnamamide
2-Propenamide, *N*-cyclododecyl-3-phenyl
RN: 59832-03-0 **MP** (°C)**:**
MW: 313.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-08	1.226E-05	ns	H350	0 0 0 0 0	

4246. $C_{21}H_{31}N_3O_2$
2-Pentoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-pentoxyquinoline-4-carboxamide
RN: 2717-02-4 **MP** (°C)**:**
MW: 357.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-05	1.895E-02	ns	B018	0 0 0 0 1	
5.300E-05	1.895E-02	ns	M066	0 0 0 0 1	

4247. $C_{21}H_{32}O_2$
3,20-Pregnanedione
7α-17-Dimethyltestosterone
Bolasterone
RN: 128-23-4 **MP** (°C)**:**
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-04	5.800E-02	37	H004	0 0 0 0 0	

4248. $C_{21}H_{32}O_2$
7α,17-Dimethyl-19-nortestosterone
RN: **MP** (°C)**:**
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-04	4.540E-02	37	H004	0 0 0 0 0	

4249. $C_{21}H_{32}O_2$
Pregnenolone
3β-Hydroxy-5-pregnen-20-one
5-Pregnen-3β-ol-20-one
3β-Hydroxypregn-5-en-20-one
RN: 145-13-1 **MP** (°C)**:** 193
MW: 316.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E-05	7.058E-03	37	H034	1 0 2 1 2	pH 7.4
9.479E-05	3.000E-02	amb	L434	0 0 0 0 0	
1.295E-04	4.100E-02	rt	B408	0 0 2 2 2	

4250. $C_{21}H_{32}O_3$
Androstanolone acetate
Androstan-3-one, 17-(acetyloxy)-, (5α,17β)-
Stanolone acetate
RN: 1164-91-6 **MP** (°C)**:**
MW: 332.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-01	8.884E+01	ns	B057	0 2 1 1 2	

4251. $C_{21}H_{33}NO$
2-Propenamide, *N*-dodecyl-3-phenyl-
RN: 55125-24-1 **MP** (°C)**:**
MW: 315.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-06	6.626E-04	ns	H350	0 0 0 0 0	

4252. $C_{21}H_{33}NO_7$
Lasiocarpine
(7α-Angelyloxy-5,6,7,8α-tetrahydro-3H-pyrrolizin-1-yl)methyl-2,3-dihydroxy-2-(1′-methoxyethyl)-3-methylbutyrate
RN: 303-34-4 **MP** (°C)**:** 97
MW: 411.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-02	6.754E+00	ns	I312	0 0 0 0 0	

4253. $C_{21}H_{34}O_2$
Pregnanolone
3-Deoxo-3a-hydroxy-5b-dihydroprogesterone
3a,5b-Tetrahydroprogesterone
3a-Hydroxy-5b-pregnan-20-one
Pregnan-3a-ol-20-one
3a,5b-Pregnanolone
RN: 128-20-1 **MP** (°C)**:**
MW: 318.50 **BP** (°C)**:** 431.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-05	8.000E-03	rt	B408	0 0 2 2 2	

4254. $C_{21}H_{34}O_3$
Tetradecyl *p*-hydroxybenzoate
Tetradecyl 4-hydroxybenzoate
RN: 71177-53-2 **MP** (°C)**:**
MW: 334.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-03	3.639E-01	25	D081	1 2 2 1 2	

4255. $C_{21}H_{35}NO_3$
4-Octoxybenzoic acid-2-(diethyl-amino)ethyl ester
RN: 38973-76-1 **MP** (°C)**:**
MW: 349.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.398E-02	ns	M066	0 0 0 0 1	

4256. $C_{21}H_{36}O_4$
4-Nonylphenol triethoxylate
Ethanol, 2-[2-[2-(4-nonylphenoxy)ethoxy]ethoxy]-
RN: 51437-95-7 **MP** (°C)**:**
MW: 352.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-05	5.880E-03	20.5	A335	0 0 0 0 0	
1.670E-05	5.887E-03	20.5	A335	0 0 0 0 0	

4257. $C_{21}H_{40}O_4$
α-Monoolein
1-Monoolein
Glycerol monooleate
9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol
1-Oleoyl-*sn*-glycerol
RN: 25496-72-4 **MP** (°C)**:**
MW: 356.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<3.57E-03	30	O321	0 0 0 0 0	

4258. $C_{21}H_{44}$
3-Methyleicosane
18-Methyleicosane
RN: 6418-46-8 **MP** (°C)**:**
MW: 296.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.294E-13	1.570E-10	23	C332	0 0 0 0 0	

4259. $C_{21}H_{44}$
2-Methyleicosane
19-Methyleicosane
RN: 1560-84-5 **MP** (°C)**:**
MW: 296.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.091E-13	1.510E-10	23	C332	0 0 0 0 0	

4260. $C_{22}H_{12}$
Indeno(1,2,3-cd)pyrene
Indeno[1,2,3-cd]pyrene
o-Phenylenepyrene
RN: 193-39-5 **MP** (°C)**:** 162.5
MW: 276.34 **BP** (°C)**:** 536

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.876E-10	1.900E-07	ns	W302	0 0 0 0 1	

4261. $C_{22}H_{12}$
Benzo[g,h,i]perylene
Benz[g,h,i]perylene
RN: 191-24-2 **MP** (°C)**:** 279
MW: 276.34 **BP** (°C)**:** >500

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.958E-10	1.370E-07	25	D406	1 2 2 2 2	
6.500E-10	1.796E-07	25	K123	1 0 2 2 1	
9.409E-10	2.600E-07	25	M064	1 1 2 2 1	
9.400E-10	2.598E-07	25	M342	1 0 1 1 1	
9.409E-10	2.600E-07	ns	M344	0 0 0 0 1	
2.533E-09	7.000E-07	ns	W302	0 0 0 0 0	

4262. $C_{22}H_{14}$
Picene
1,2,7,8-Dibenzphenanthrene
3,4-Benzchrysene
RN: 213-46-7 **MP** (°C)**:** 366
MW: 278.36 **BP** (°C)**:** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-08	4.315E-06	20	E009	1 0 0 1 2	
8.981E-09	2.500E-06	27	D003	1 0 0 1 1	

4263. $C_{22}H_{14}$
1,2:3,4-Dibenzanthracene
RN: 215-58-7 **MP** (°C)**:** 205
MW: 278.36 **BP** (°C)**:** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-09	1.600E-06	25	B319	2 0 1 2 1	
8.200E-08	2.283E-05	25	K123	1 0 2 2 1	

4264. $C_{22}H_{14}$
1,2:7,8-Dibenzanthracene
Dibenz[a,j]anthracene
Dinaphthanthracene
RN: 224-41-9 **MP** (°C)**:** 196
MW: 278.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-08	8.629E-06	25	K123	1 0 2 2 1	
4.311E-08	1.200E-05	27	D003	1 0 0 1 1	

4265. $C_{22}H_{14}$
1,2:5,6-Dibenzanthracene
1,2,5,6-Dibenzanthracene
RN: 53-70-3 **MP** (°C)**:** 266
MW: 278.36 **BP** (°C)**:** 524

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.945E-09	2.490E-06	24	H106	1 0 2 2 2	
7.904E-09	2.200E-06	25	B319	2 0 1 2 2	
2.150E-09	5.985E-07	25	K001	2 2 2 2 2	
1.100E-07	3.062E-05	25	K123	1 0 2 2 1	*sic*
8.945E-09	2.490E-06	25	M156	1 2 1 1 2	
1.800E-09	5.010E-07	25	M342	1 0 1 1 2	
1.796E-09	5.000E-07	27	D003	1 0 0 1 1	

4266. $C_{22}H_{16}F_3N_3$
Fluotrimazole
1H-1,2,3-Triazole, 1-[diphenyl[3-(trifluoromethyl)phenyl]methyl]-
RN: 57381-79-0 **MP** (°C)**:** 132
MW: 379.39 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E-09	1.500E-06	20	M161	1 0 0 0 1	

4267. $C_{22}H_{16}O_8$
Ethyl biscoumacetate
Tromexan
RN: 548-00-5 **MP** (°C)**:** 154
MW: 408.37 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.179E-04	8.900E-02	20	K028	2 1 2 1 2	pH 3.8, form I
3.747E-04	1.530E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.179E-04	8.899E-02	20	M042	1 0 0 0 1	pH 3.8, form I, mp 172-182 C
3.761E-04	1.536E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 153-160 C

4268. $C_{22}H_{17}ClN_2$
Clotrimazole
1-(*o*-Chloro-α,α-diphenylbenzyl)imidazole
1-[α-(2-Chlorophenyl)benzhydryl]imidazole
Lotrimin
RN: 23593-75-1 **MP** (°C)**:** 147–149
MW: 344.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.90E-05	<1.00E-02	25	H328	0 0 0 0 0	
8.700E-05	3.000E-02	amb	L434	0 0 0 0 0	

4269. $C_{22}H_{18}N_2O_4S$
Hydantoin, 5,5-diphenyl-1-(*o*-tolylsulfonyl)-
1-(*o*-Methylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-41-9 **MP** (°C)**:**
MW: 406.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-06	7.600E-04	37	F183	1 0 1 1 2	intrinsic

4270. $C_{22}H_{18}N_2O_5S$
1-(*p*-Methoxylbenzenesulfonyl)-5,5-diphenyl-hydantoin
RN: 24759-37-3 **MP** (°C)**:**
MW: 422.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-06	5.100E-04	37	F183	1 0 1 1 2	intrinsic

4271. $C_{22}H_{19}Br_2NO_3$
Deltamethrin
3-(2,2-Dibromoethenyl)-2,2-dimethylcyclopropanecarboxylic acid, cyano(3-phenoxyphenyl) methyl ester
RN: 52918-63-5 **MP** (°C)**:** 98–101
MW: 505.22 **BP** (°C)**:** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-09	2.000E-06	25	M364	1 0 0 0 1	
3.959E-09	2.000E-06	ns	V414	0 0 0 0 0	

4272. $C_{22}H_{19}F_6NOS$
α-Piperidyl-3,6-bis(trifluoromethyl)-9-phenanthrenemethanol
RN: 31817-24-0 **MP** (°C)**:** 215
MW: 459.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E-05	7.500E-03	25	A013	1 0 2 2 0	average

4273. $C_{22}H_{20}$
10-Butyl-1,2-benzanthracene
RN: 188124-94-9 **MP** (°C)**:** 97
MW: 284.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-08	8.000E-06	27	D003	1 0 0 1 1	

4274. $C_{22}H_{20}Cl_2N_2O_3$
Benzofenap
2-((4-(2,4-Dichloro-3-methylbenzoyl)-1,3-dimethyl-1H-pyrazol-5-yl)oxy)-1-(4-methylphenyl) ethanone
RN: 82692-44-2 **MP** (°C)**:**
MW: 431.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-07	1.303E-04	ns	R427	0 0 0 0 0	

4275. $C_{22}H_{20}O_{13}$
Carminic acid
Carmine
Carminsaeure
RN: 1260-17-9 **MP** (°C)**:**
MW: 492.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.637E-03	1.298E+00	rt	D021	0 0 1 1 1	

4276. $C_{22}H_{22}ClN_3O_5$

Propaquizafop
2-[(Isopropylideneamino)oxy]ethyl (*R*)-2-[*p*-[(6-chloro-2-quinoxalinyl)oxy]phenoxy]-propionate
(*R*)-2-{[(1 Methylethylidene)amino]oxy}ethyl 2-{4-[(6-chloro-2-quinoxalinyl)oxy]phenoxy} propanoate
Agil
Shogun
RO 17-3664
RN: 111479-05-1 **MP** (°C)**:**
MW: 443.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-06	6.270E-04	ns	R427	0 0 0 0 0	

4277. $C_{22}H_{22}FN_3O_2$

Droperidol
2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro-
Sintodril
Neurolidol
R 4749
RN: 548-73-2 **MP** (°C)**:**
MW: 379.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-05	4.100E-03	30	P044	0 0 0 0 0	

4278. $C_{22}H_{22}N_2O_4$

N,*N*′-Dibutyl-1,4,5,8-naphthalenediimide
Benzo[*lmn*][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-dibutyl-
1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide, *N*,*N*′-dibutyl-
RN: 17655-95-7 **MP** (°C)**:**
MW: 378.43 **BP** (°C)**:** 572.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.892E-06	23	B410	2 1 2 2 2	

4279. $C_{22}H_{22}N_2O_8$
Methacycline base
Oxytetracycline, 6-methylene-
Tri-methacycline
Rondomycin
RN: 914-00-1 **MP** (°C)**:**
MW: 442.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.706E-02	7.548E+00	21	M044	2 0 2 2 2	

4280. $C_{22}H_{22}N_4O_6$
Benzoyl-mitomycin C
RN: **MP** (°C)**:**
MW: 438.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	4.384E-03	25	M316	1 1 1 1 2	

4281. $C_{22}H_{23}ClN_2O_8$
Chlortetracycline
7-Chlortetracycline
Acronize PD
Acronize
RN: 57-62-5 **MP** (°C)**:**
MW: 478.89 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-03	6.300E-01	25	B191	1 0 0 0 1	
2.297E-03	1.100E+00	37	M104	1 2 1 1 0	form II, EFG, recrystallized
1.566E-03	7.500E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized
2.088E-04	1.000E-01	37	M105	1 2 1 1 0	EFG

4282. $C_{22}H_{23}NO_3$
Fenpropanate
Danitol
Herald
WL 41706
Miothrin
2,2,3,3-Tetramethylcyclopropane carboxylic acid, cyano(3-phenoxyphenyl)methyl ester
RN: 39515-41-8 **MP** (°C)**:**
MW: 349.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-08	1.424E-05	ns	R427	0 0 0 0 0	

4283. $C_{22}H_{23}NO_7$
Noscapine
Narcotine
O-Methylnarcotoline
Opianin
Opian
RN: 128-62-1 **MP** (°C)**:** 176
MW: 413.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.654E-02	15	K059	2 2 2 0 0	
7.327E-04	3.029E-01	25	D004	0 0 0 0 0	
7.256E-04	3.000E-01	30	A073	1 1 1 1 0	
1.693E-03	7.000E-01	40	A073	1 1 1 1 0	
2.419E-03	1.000E+00	50	A073	1 1 1 1 1	
2.419E-03	1.000E+00	60	A073	1 1 1 1 1	
2.419E-03	1.000E+00	70	A073	1 1 1 1 1	
2.419E-03	1.000E+00	80	A073	1 1 1 1 1	
3.628E-03	1.500E+00	90	A073	1 1 1 1 1	
4.838E-03	2.000E+00	100	A073	1 1 1 1 1	

4284. $C_{22}H_{24}ClN_5O_2$
Domperidone
5-Chloro-1-[1-[3-(2-oxo-1-benzimidazolinyl)propyl]-4-piperidyl]-2-benzimidazolinone
RN: 57808-66-9 **MP** (°C)**:** 242.5
MW: 425.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-05	1.710E-02	22	J420	0 0 0 0 0	pH6.5

4285. $C_{22}H_{24}N_2O_8$

Tetracycline
Achromycin V
Sumycin
Robitet
Panmycin

RN: 60-54-8 **MP** (°C)**:** 176dec
MW: 444.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.900E-04	4.400E-01	25	B191	1 0 0 0 1	neutral pH
5.200E-04	2.311E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
5.700E-04	2.533E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
2.655E-03	1.180E+00	29	N031	1 2 2 2 0	EFG, pH 5.0
7.600E-04	3.378E-01	30	L069	1 0 1 1 0	EFG
1.777E-03	7.900E-01	35	N031	1 2 2 2 0	EFG, pH 5.0
7.875E-02	3.500E+01	37	M104	1 2 1 1 2	form II, recrystallized
6.232E-02	2.770E+01	37	M104	1 2 1 1 2	form I, recrystallized
6.478E-04	2.879E-01	ns	N302	0 2 1 2 2	

4286. $C_{22}H_{24}N_2O_8.H_2O$

Doxycycline (monohydrate)
Doxylin
Monodox
Vibra-tabs
Doxy-caps
Vibramycin

RN: 564-25-0 **MP** (°C)**:** 201dec
MW: 462.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.362E-03	6.300E-01	25	B132	2 1 1 1 0	EFG

4287. $C_{22}H_{24}N_2O_9$

Oxytetracycline
Glomycin
Hydroxytetracycline
Riomitsin
Terrafungine
Stevacin

RN: 79-57-2 **MP** (°C)**:** 184
MW: 460.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.234E-04	1.950E-01	20	L051	1 0 0 0 2	
9.990E-04	4.600E-01	25	B191	1 0 0 0 1	neutral pH

(*continued*)

4287. $C_{22}H_{24}N_2O_9$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	2.210E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
6.798E-04	3.130E-01	25	H005	1 0 1 2 2	Ph 5.8
5.000E-04	2.302E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
6.515E-04	3.000E-01	29	N031	1 2 2 2 0	EFG, pH 5.0
8.687E-04	4.000E-01	37	M104	1 2 1 1 0	form II, EFG, recrystallized
6.515E-04	3.000E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized

4288. $C_{22}H_{24}N_4O_5$

Benzyl-mitomycin C

RN: **MP** (°C)**:**

MW: 424.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	6.324E-01	25	M316	1 1 1 1 2	

4289. $C_{22}H_{24}N_4O_5S$

Methanesulfonamide, *N*-[1′-[2-(2,1,3-benzoxadiazol-5-yl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4′-piperidin]-6-yl]-

Methanesulfonamide, *N*-[1′-[2-(5-benzofurazanyl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4′-piperidin]-6-yl]-

RN: **MP** (°C)**:**

MW: 456.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.752E-05	8.000E-03	22	D405	1 1 2 2 2	Intrinsic

4290. $C_{22}H_{25}NO_6$

Colchicine

Colchicin

RN: 64-86-8 **MP** (°C)**:**

MW: 399.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-02	3.846E+01	20	D041	1 0 0 0 0	
1.088E-01	4.348E+01	25	D004	0 0 0 0 0	
8.261E-02	3.300E+01	ns	K444	0 0 0 0 0	

4291. $C_{22}H_{26}F_3N_3OS$
Fluphenazine
Permitil
Modecate
Prolixin
RN: 69-23-8 **MP** (°C)**:** <25
MW: 437.53 **BP** (°C)**:** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-05	3.106E-02	37	F011	1 0 1 1 1	pH 7.4

4292. $C_{22}H_{26}N_2O_9$
Doxycycline
4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamide monohydrate
Doryx
Doxylin
Monodox
Vibramycin
RN: 564-25-0 **MP** (°C)**:**
MW: 462.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E+00	1.087E+03	25	B443	0 0 0 0 0	
2.162E-04	1.000E-01	ns	K444	0 0 0 0 0	

4293. $C_{22}H_{27}ClN_2O_4S$
Diltiazem hydrochloride
1,5-Benzothiazepin-4(5H)one,3-(acetyloxy)-5-(2-(dimethylamino)ethyl)-2,3-dihydro-2-(4-methoxyphenyl)-,
Dilacor XR
Cardizem
Cardcal
Coras
RN: 33286-22-5 **MP** (°C)**:**
MW: 450.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.131E-03	5.100E-01	25	A412	1 0 2 2 1	int

4294. $C_{22}H_{27}NO_2$
Danazol
17α-Pregna-2,4-dien-20-yno[2,3-d]isoxazol-17-ol
Danocrine
Cyclomen
RN: 17230-88-5 **MP** (°C)**:**
MW: 337.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-06	5.800E-04	25	E409	0 0 0 0 0	
1.245E-06	4.200E-04	37	S446	0 0 0 0 0	

4295. $C_{22}H_{28}F_2O_5$
Flumethasone
Flumethasonpivalate
RN: 2135-17-3 **MP** (°C)**:**
MW: 410.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.436E-06	1.000E-03	20	A067	0 0 0 0 0	

4296. $C_{22}H_{28}N_2O$
Fentanyl
1-Phenethyl-4-(phenylpropionylamino)piperidine
N-(1-Phenethyl-4-piperidyl)propionanilide
Duragesic
RN: 437-38-7 **MP** (°C)**:**
MW: 336.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.944E-04	2.000E-01	25	R338	0 0 0 0 0	
3.566E-05	1.200E-02	35	R418	0 0 0 0 0	Intrinsic

4297. $C_{22}H_{28}N_6O_3S$
Delavirdine
1-[3-[(1-Methylethyl)amino]-2-pyridinyl]-4-[[5-[(methylsulfonyl)amino]-1H-indol-2-yl]carbonyl] piperazine
1-(5-Methanesulfonamido-1H-indol-2-ylcarbonyl)-4-[3-(1-methylethylamino)pyridinyl]piperazine
1-[3-(Isopropylamino)-2-pyridyl]-4-[(5-methanesulfonamidoindol-2-yl)carbonyl]piperazine
RN: 136817-59-9 **MP** (°C)**:**
MW: 456.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.571E-02	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic

4298. $C_{22}H_{28}O_3$
Canrenone
17-Hydroxy-3-oxo-17α-pregna-4,6-diene-21-carboxylic acid lactone
RN: 976-71-6 **MP** (°C)**:** 149-151
MW: 340.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-07	2.724E-04	25	G017	1 0 1 0 0	EFG
8.100E-05	2.758E-02	37	C004	0 0 0 0 0	*sic*
8.958E-07	3.050E-04	37	O306	1 0 2 2 2	
6.374E-07	2.170E-04	rt	O306	0 0 2 2 2	

4299. $C_{22}H_{28}O_3$
Norethindrone acetate
Norethisterone acetate
RN: 51-98-9 **MP** (°C)**:** 161
MW: 340.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.288E-06	3.162E-03	10	L078	1 0 1 2 0	EFG
1.312E-05	4.467E-03	20	L078	1 0 1 2 0	EFG
1.570E-05	5.345E-03	25	H099	1 0 2 2 2	
1.652E-05	5.623E-03	25	L078	1 0 1 2 2	
1.853E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
2.937E-05	1.000E-02	40	L078	1 0 1 2 0	EFG

4300. $C_{22}H_{29}FO_4$
Fluorometholone
9-Fluoro-11β,17-dihydroxy-6α-methylpregna-1,4-diene-3,20-dione
21-Desoxy-9α-fluoro-6α-methyl-prednisolone
RN: 426-13-1 **MP** (°C)**:**
MW: 376.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.968E-05	3.000E-02	25	G008	1 2 1 1 0	

4301. $C_{22}H_{29}FO_5$
Betamethasone
Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11β,16β)-
RN: 378-44-9 **MP** (°C)**:** 230
MW: 392.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-04	5.800E-02	25	K003	2 1 1 1 1	
1.936E-04	7.599E-02	25	P096	0 0 0 0 0	

(*continued*)

4301. $C_{22}H_{29}FO_5$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	5.887E-02	30	O321	0 0 0 0 0	
1.529E-04	6.000E-02	30	O321	0 0 0 0 0	
1.605E-04	6.301E-02	37	C400	2 0 2 2 2	
1.605E-04	6.300E-02	ns	B404	0 2 1 1 0	
1.575E-04	6.180E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

4302. $C_{22}H_{29}FO_5$

Dexamethasone

Dexamethasone alcohol

RN: 50-02-2 **MP** (°C)**:** 262

MW: 392.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	3.218E-02	10	B012	2 0 1 1 0	
1.580E-04	6.201E-02	20	B012	2 0 1 1 0	
2.800E-04	1.099E-01	23	L345	1 0 1 1 2	
2.270E-04	8.909E-02	25	B012	2 0 1 1 0	
2.140E-04	8.399E-02	25	K003	2 1 1 1 1	
3.083E-04	1.210E-01	25	K021	1 2 2 2 1	
2.548E-04	1.000E-01	25	P312	0 0 0 0 0	
2.520E-04	9.890E-02	30	B012	2 0 1 1 0	
2.344E-04	9.200E-02	37	C400	2 0 2 2 2	
2.955E-04	1.160E-01	37	D026	0 0 0 0 0	
3.560E-04	1.397E-01	40	B012	2 0 1 1 0	
4.600E-04	1.805E-01	50	B012	2 0 1 1 0	
4.077E-04	1.600E-01	amb	L434	0 0 0 0 0	
2.548E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.707E-04	6.700E-02	ns	N302	0 2 1 2 1	

4303. $C_{22}H_{29}NO_7S_2$

Methyl *O*-acetyl-3-(acetyloxy)-*N*-{5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: **MP** (°C)**:**

MW: 483.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.817E-04	2.329E-01	ns	S453	0 0 0 0 0	

4304. $C_{22}H_{30}ClNO_2$

Propoxyphene hydrochloride
D-Propoxyphene hydrochloride
RN: 1639-60-7 **MP** (°C)**:**
MW: 375.94 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.842E-06	3.700E-03	25	A412	1 0 2 2 1	int

4305. $C_{22}H_{30}Cl_2N_{10}$

Chlorhexidin
Chlorhexidine
bis(5-(*p*-Chlorophenyl)biguanidinio)hexane
RN: 55-56-1 **MP** (°C)**:**
MW: 505.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.583E-04	7.999E-02	20	D341	0 0 0 0 0	
8.309E-05	4.200E-02	22.5	G301	0 0 0 0 0	

4306. $C_{22}H_{30}N_2O_2$

Aspidospermine
Aspidospermidine, 1-acetyl-17-methoxy-
RN: 466-49-9 **MP** (°C)**:** 208
MW: 354.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.701E-04	1.666E-01	c	D004	0 0 0 0 0	

4307. $C_{22}H_{30}N_2O_2S$

Sufentanil
N-[4-(Methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidyl]propionanilide
Sufenta
RN: 56030-54-7 **MP** (°C)**:**
MW: 386.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-04	7.600E-02	25	R338	0 0 0 0 0	
3.363E-06	1.300E-03	35	R418	0 0 0 0 0	Intrinsic

4308. $C_{22}H_{30}O_5$
Methylprednisolone
6α-Methylprednisolone
Medrol
Solumedrol
Metrisone
Promacortine
RN: 83-43-2 **MP** (°C)**:** 232.5
MW: 374.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.204E-04	1.200E-01	25	A014	1 0 1 1 0	EFG
2.403E-04	9.000E-02	25	A014	1 0 1 1 0	EFG, pH 5.0
2.534E-03	9.491E-01	25	G008	1 2 1 1 1	
3.445E-04	1.290E-01	25	K021	1 2 2 2 1	
1.335E-04	5.000E-02	27.14	H026	1 0 2 1 0	EFG, form I
1.923E-04	7.199E-02	30.0	H010	2 2 1 1 1	
4.273E-04	1.600E-01	31.72	H026	1 0 2 1 0	EFG, form II
3.124E-04	1.170E-01	37	H004	0 0 0 0 0	polymorph I
3.765E-04	1.410E-01	37	H004	0 0 0 0 0	polymorph II
5.341E-04	2.000E-01	40.32	H026	1 0 2 1 0	EFG, form II
2.937E-04	1.100E-01	40.32	H026	1 0 2 1 0	EFG, form I
4.273E-04	1.600E-01	51.52	H026	1 0 2 1 0	EFG, form I
1.362E-03	5.100E-01	81.45	H026	1 0 2 1 0	EFG, form II
1.068E-03	4.000E-01	81.45	H026	1 0 2 1 0	EFG, form I
2.670E-04	1.000E-01	ns	M169	0 0 0 0 1	

4309. $C_{22}H_{30}O_6$
5,16-β-Dihydroxy-6-β-methyl-3,11-dioxo-5-α-pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester
U-20235
RN: **MP** (°C)**:**
MW: 390.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.402E-04	2.500E-01	ns	K029	0 0 2 1 1	

4310. $C_{22}H_{32}O_3$
Nandrolone butyrate
RN: **MP** (°C)**:**
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-05	5.030E-03	37	C026	0 0 0 0 0	

4311. $C_{22}H_{32}O_3$
Methyltestosterone acetate
17-α-Methyltestosterone acetate
RN: 1099-79-2 **MP** (°C)**:** 164
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-05	4.926E-03	25	H099	1 0 2 2 2	
5.196E-06	1.790E-03	ns	B057	0 2 1 1 2	

4312. $C_{22}H_{32}O_3$
5,6-Dehydroisoandrosterone propionate
RN: 1167-87-9 **MP** (°C)**:**
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-05	8.320E-03	ns	B057	0 2 1 1 2	

4313. $C_{22}H_{32}O_3$
Testosterone propionate
17-(1-Oxopropoxy)-(17β)-androst-4-en-3-one
Testosterone-17-propionate
Agovirin
Androsan
Androgen
RN: 57-85-2 **MP** (°C)**:** 120
MW: 344.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.891E-02	20	F012	1 0 1 1 1	
4.300E-06	1.481E-03	25	J004	1 0 1 1 2	
5.806E-06	2.000E-03	25	K003	2 1 1 1 1	
6.096E-06	2.100E-03	30	T005	2 0 2 2 1	
1.060E-05	3.652E-03	37.50	B054	1 0 1 1 2	
4.296E-06	1.480E-03	ns	B057	0 2 1 1 2	

4314. $C_{22}H_{33}N_3O_2$
2-Hexoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-hexoxyquinoline-4-carboxamide
RN: 2717-03-5 **MP** (°C)**:**
MW: 371.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-06	2.489E-03	ns	B018	0 0 0 0 1	
6.700E-06	2.489E-03	ns	M066	0 0 0 0 1	

4315. $C_{22}H_{34}Cl_2O_3$
2,4-Dichlorophenoxyacetic acid *n*-tetradecyl ester
RN: 65267-96-1 **MP** (°C)**:**
MW: 417.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-05	4.848E-03	ns	M120	0 0 1 1 2	

4316. $C_{22}H_{34}N_6O_4$
2,5-Diaziridinyl-3,6-di(1′-piperazineethanol)-1,4-benzoquinone
RN: 59886-40-7 **MP** (°C)**:** 170
MW: 446.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-02	2.000E+01	rt	C317	0 0 0 0 0	

4317. $C_{22}H_{34}O_3$
Androstanolone propionate
Androstan-3-one, 17-(1-oxopropoxy)-, (5α,17β)-
RN: 855-22-1 **MP** (°C)**:**
MW: 346.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E-06	6.200E-04	ns	B057	0 2 1 1 2	

4318. $C_{22}H_{35}NO_3$
Acetaminophen myristate
Acetaminophen tetradecanoate
RN: 54942-39-1 **MP** (°C)**:** 114
MW: 361.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-05	6.000E-03	25	B010	1 1 1 1 0	

4319. $C_{22}H_{37}NO_2$
Anandamide
Arachidonoylethanolamide
AEA
RN: 94421-68-8 **MP** (°C)**:**
MW: 347.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.188E-06	4.130E-04	25	J414	0 0 0 0 0	Intrinsic

4320. $C_{22}H_{38}O_5$
4-Octylphenol tetraethoxylate
Ethanol, 2-[2-[2-[2-(4-octylphenoxy)ethoxy]ethoxy]ethoxy]-
RN: 51437-92-4 **MP** (°C)**:**
MW: 382.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.404E-05	2.450E-02	20.5	A335	0 0 0 0 0	
6.410E-05	2.452E-02	20.5	A335	0 0 0 0 0	

4321. $C_{22}H_{39}O_3P$
Diisooctyl phenyl phosphonate
RN: **MP** (°C)**:**
MW: 382.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.61E-04	<1.00E-01	25	B070	1 2 0 1 0	

4322. $C_{22}H_{39}O_3P$
Dioctyl phenyl phosphonate
Di-*n*-octyl phenylphosphonate
DOPP
RN: 1754-47-8 **MP** (°C)**:**
MW: 382.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.23E-04	<2.00E-01	25	B070	1 2 0 1 0	

4323. $C_{22}H_{42}O_4$
Dioctyl adipate
bis(2-Ethylhexyl) adipate
RN: 103-23-1 **MP** (°C)**:**
MW: 370.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.095E-06	3.000E-03	25	F067	1 0 2 2 1	

4324. $C_{22}H_{43}N_5O_{13}$
Amikacin
Antibiotic BB-K8
RN: 37517-28-5 **MP** (°C)**:** 203
MW: 585.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-01	1.850E+02	25	K044	1 0 0 0 2	pH 10.4

4325. $C_{23}H_{16}O_6$
Pamoic acid
4,4′-Methylenebis[3-hydroxy-2-naphthalenecarboxylic acid]
3,3′-Dihydroxy-4,4′-methylenedi-2-naphthoic acid
Embonic acid
RN: 130-85-8 **MP** (°C)**:**
MW: 388.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	1.087E+02	ns	F007	0 0 0 0 1	

4326. $C_{23}H_{18}F_2N_4O$
α-(2,4-Difluorophenyl)-α-(1-2-(2-pyridyl)phenylethenyl)-1H-1,2,4-triazole-1-ethanol
XD405
RN: 124669-93-8 **MP** (°C)**:**
MW: 404.42 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.418E-06	3.000E-03	22	M372	1 2 1 1 1	intrinsic

4327. $C_{23}H_{20}N_2O_2S$
G-1
p-Phenylthioethylphenylbutazone
1,2-Diphenyl-4-(2-phenylthioethyl)-3,5-pyrazolidinedione
RN: 3736-92-3 **MP** (°C)**:**
MW: 388.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.118E-03	1.600E+00	ns	B158	0 0 0 0 1	pH 7.0

4328. $C_{23}H_{20}N_2O_3S$
Sulfinpyrazone
Sulfoxyphenyl pyrazolidine
Sulfinpyrazole
1,2-Diphenyl-4-(2-(phenylsulfinyl)ethyl)-3,5-pyrazolidinedione
Anturane
RN: 57-96-5 **MP** (°C)**:**
MW: 404.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.431E-03	2.601E+00	22	J420	0 0 0 0 0	pH6.5

4329. $C_{23}H_{22}$
10-Amyl-1,2-benzanthracene
RN: 188124-96-1 **MP** (°C)**:**
MW: 298.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.681E-09	8.000E-07	27	D003	1 0 0 1 0	

4330. $C_{23}H_{22}O_6$
Rotenone
Tubatoxin
Derris
1,2,12,12α-Tetrahydro-2α-isopropenyl-8,9-dimethoxy(1)benzopyrano(3,4-b)furo(2,3-h)(1) benzopyran-6(6α H)-one
RN: 83-79-4 **MP** (°C)**:** 163
MW: 394.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-07	1.700E-04	25	C100	1 0 2 1 1	
3.803E-05	1.500E-02	100	M161	1 0 0 0 1	

4331. $C_{23}H_{23}NO$
Trifenmorph
Frescon
N-Tritylmorpholine
RN: 1420-06-0 **MP** (°C)**:** 175
MW: 329.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E-08	2.000E-05	20	M161	1 0 0 0 1	

4332. $C_{23}H_{24}N_4O_2$
Diantipyrylmethane
4,4′-Methylenediantipyrine
4,4′-Diantipyrylmethane
RN: 1251-85-0 **MP** (°C)**:** 182
MW: 388.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-03	4.390E-01	20	P054	0 0 0 0 0	
1.132E-03	4.398E-01	20	P054	0 0 0 0 0	

4333. $C_{23}H_{24}N_4O_6$
Benzylcarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 452.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	1.014E+00	25	M316	1 1 1 1 2	

4334. $C_{23}H_{24}N_4O_7$
Benzyloxycarbonyl-mitomycin C
RN: **MP** (°C)**:**
MW: 468.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-04	2.436E-01	25	M316	1 1 1 1 2	

4335. $C_{23}H_{24}N_4S_2$
Dithiodiantipyrinylmethane
3H-Pyrazole-3-thione, 4,4′-methylenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 53799-78-3 **MP** (°C)**:** 166
MW: 420.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.103E-01	ns	D087	0 2 0 0 1	

4336. $C_{23}H_{25}N$
Fendiline
RN: 13042-18-7 **MP** (°C)**:**
MW: 315.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.389E-06	2.331E-03	22.5	B440	0 0 0 0 0	

4337. $C_{23}H_{26}FN_3O_2$
Spiperone
8-[4-(4-Fluorophenyl)-4-oxobutyl]-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one
RN: 749-02-0 **MP** (°C)**:** 192 C
MW: 395.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.091E-05	3.200E-02	22	J420	0 0 0 0 0	pH6.5

4338. $C_{23}H_{26}N_2O_4$
Brucine
Brucin
RN: 357-57-3 **MP** (°C)**:** 178
MW: 394.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.112E-03	3.200E+00	15	F300	1 0 0 0 1	
1.330E-03	5.247E-01	15	K059	2 2 2 0 2	
1.698E-02	6.700E+00	100	F300	1 0 0 0 1	
1.267E-03	4.998E-01	rt	D021	0 0 1 1 1	

4339. $C_{23}H_{26}N_2O_4.4H_2O$
Brucine (tetrahydrate)
Strychnidin-10-one, 2,3-dimethoxy-, tetrahydrate
RN: 5892-11-5 **MP** (°C)**:** 105
MW: 466.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.677E-03	3.115E+00	c	D004	0 0 0 0 0	
1.420E-02	6.623E+00	h	D004	0 0 0 0 0	

4340. $C_{23}H_{26}O_3$
Phenothrin
(3-Phenoxylphenyl)methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate
Sumithrin
3-Phenoxybenzyl D-*cis* and *trans*-2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate
RN: 26002-80-2 **MP** (°C)**:** <25
MW: 350.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	2.000E-03	30	M161	1 0 0 0 0	

4341. $C_{23}H_{27}ClO_4$
Delmadinone acetate
Pregna-1,4,6-triene-3,20-dione, 17-(acetyloxy)-6-chloro-
RN: 13698-49-2 **MP** (°C)**:** 168
MW: 402.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-05	6.070E-03	37	K070	1 0 0 1 2	
1.134E-05	4.570E-03	ns	K070	1 0 0 1 2	

4342. $C_{23}H_{27}FN_4O_2$
Risperidal
3-(2-(4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl)ethyl)-6,7,8,9-tetrahydro-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one
Risperidone
RN: 106266-06-2 **MP** (°C)**:**
MW: 410.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	4.474E-02	25	E406	0 0 0 0 0	
<2.44E-04	<1.00E-01	rt	B435	0 0 0 0 0	

4343. $C_{23}H_{27}NO_8$
Narceine
o-Veratric acid, 6-[[6-[2-(dimethylamino)ethyl]-2-methoxy-3,4-(methylenedioxy)phenyl]acetyl]-
NIH 10760
RN: 131-28-2 **MP** (°C)**:** 138
MW: 445.47 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	5.791E-01	15	K059	2 2 2 0 1	
2.915E-03	1.299E+00	c	D004	0 0 0 0 0	
1.016E-02	4.525E+00	h	D004	0 0 0 0 0	

4344. $C_{23}H_{27}N_3O_7$
Minocycline
Dynacin
Minocin
RN: 10118-90-8 **MP** (°C)**:**
MW: 457.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-01	5.200E+01	25	B191	1 0 0 0 1	neutral pH

4345. $C_{23}H_{28}ClN_3O_2S$
Thiopropazate
1-(2-Acetoxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine
RN: 84-06-0 **MP** (°C)**:**
MW: 446.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	8.920E-03	24	G022	2 0 1 1 1	

4346. $C_{23}H_{28}ClN_3O_5S$
Glyburide
HB 419
Glibenclamide
Diabeta
1-((*p*-(2-(5-Chloro-*o*-anisamido)ethyl)phenyl)-sulfonyl)-3-cyclohexylurea
RN: 10238-21-8 **MP** (°C)**:** 169
MW: 494.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-05	5.615E-03	22	M382	2 1 1 1 1	average of 2
6.275E-05	3.100E-02	25	G088	1 1 1 1 0	
1.000E-05	4.940E-03	25	Z410	0 0 0 0 0	EFG
8.097E-06	4.000E-03	27	H093	1 0 1 1 0	
2.024E-05	1.000E-02	ns	K444	0 0 0 0 0	

4347. $C_{23}H_{28}O_7$
Prednisone acetate
Pregna-1,4-diene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-
RN: 125-10-0 **MP** (°C)**:**
MW: 416.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.522E-05	2.300E-02	25	K003	2 1 1 1 1	

4348. $C_{23}H_{29}ClFN_3O_4$
Cisapride
4-Amino-5-chloro-*N*- [1-[3-(4-fluorophenoxy)propyl]-3-methoxy-4-piperidyl]-2-methoxy-benzamide
RN: 81098-60-4 **MP** (°C)**:**
MW: 465.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	9.319E-03	30	A417	0 0 0 0 0	pH 8.2
4.000E-04	1.864E-01	30	A417	0 0 0 0 0	pH 3.6

4349. $C_{23}H_{31}Cl_2NO_3$
Estramustine
Estradiol 3-[bis(2-chloroethyl)carbamate]
3-[bis(2-Chloroethyl)carbamate
RN: 2998-57-4 **MP** (°C)**:**
MW: 440.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.27E-06	~1.00E-03	30	L334	1 0 1 1 0	

4350. $C_{23}H_{31}FO_6$
9α-Fluorohydrocortisone acetate
Pregn-4-ene-3,20-dione, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β)-
RN: 514-36-3 **MP** (°C)**:**
MW: 422.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-04	5.400E-02	25	K021	1 2 2 2 1	

4351. $C_{23}H_{31}N_5O_4$
Benzoic acid, 3-[(dipropylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-71-1 **MP** (°C)**:**
MW: 441.53 **BP** (°C)**:** 674.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E-04	1.300E-01	21	B419	1 1 2 2 1	int

4352. $C_{23}H_{31}O_7$
Cortisone-21-hemi-succinate
RN: **MP** (°C)**:**
MW: 419.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.768E-04	2.000E-01	ns	E307	0 0 0 0 0	

4353. $C_{23}H_{32}O_2$
Medrogestone
Pregna-4,6-diene-3,20-dione, 6,17-dimethyl-
RN: 977-79-7 **MP** (°C)**:** 144
MW: 340.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.345E-06	1.820E-03	25	L033	1 0 2 1 2	

4354. $C_{23}H_{32}O_4$
Deoxycorticosterone acetate
Pregn-4-ene-3,20-dione, 21-(acetyloxy)-
RN: 56-47-3 **MP** (°C)**:** 156
MW: 372.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-05	4.000E-03	25	K003	2 1 1 1 1	

4355. $C_{23}H_{32}O_6$
Hydrocortisone acetate
Hydrocortisone-21-acetate
Cortisol acetate
Cortisol 21-acetate
RN: 50-03-3 **MP** (°C)**:** 223dec
MW: 404.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.486E-05	1.410E-02	25	C037	2 1 2 2 2	
1.555E-05	6.290E-03	25	H098	1 0 2 0 2	
1.555E-05	6.290E-03	25	H320	0 0 0 0 0	
1.550E-05	6.270E-03	25	H320	0 0 0 0 0	
2.472E-05	1.000E-02	25	K003	2 1 1 1 1	
3.461E-05	1.400E-02	25	K021	1 2 2 2 1	
2.472E-05	1.000E-02	25	M023	1 0 2 1 0	
2.472E-05	1.000E-02	ns	M169	0 0 0 0 1	
1.904E-05	7.700E-03	ns	N323	0 0 0 0 0	

4356. $C_{23}H_{34}O_3$
Testosterone butyrate
Androst-4-en-3-one, 17-(1-oxobutoxy)-, (17bet)-
RN: 3410-54-6 **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.406E-06	5.039E-04	25	J004	1 0 1 1 2	
1.403E-06	5.030E-04	ns	B057	0 2 1 1 2	

4357. $C_{23}H_{34}O_3$
5,6-Dehydroisoandrosterone butyrate
Androst-5-en-17-one, 3-(1-oxobutoxy)-, (3β)-
RN: 15253-51-7 **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.231E+00	4.413E+02	ns	B057	0 2 1 1 2	

4358. $C_{23}H_{34}O_3$
17-α-Methyltestosterone propionate
RN: **MP** (°C)**:**
MW: 358.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.845E-06	1.020E-03	ns	B057	0 2 1 1 2	

4359. $C_{23}H_{34}O_4$
Digitoxigenin
Card-20(22)-enolide, 3,14-dihydroxy-, (3β,5β)-
RN: 143-62-4 **MP** (°C)**:**
MW: 374.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.124E-02	30	O321	0 0 0 0 0	

4360. $C_{23}H_{35}NOS$
5-Pregnene-20-one-3-spiro-2′-(1′,2′-thiazolidine)
RN: **MP** (°C)**:** 127–136
MW: 373.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.34E-05	~5.00E-03	ns	B199	0 0 0 0 0	

4361. $C_{23}H_{36}N_2O_2$
Finasteride
Proscar
RN: 98319-26-7 **MP** (°C)**:**
MW: 372.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-04	4.000E-02	amb	L434	0 0 0 0 0	

4362. $C_{23}H_{36}O_3$
Androstanolone butyrate
Androstan-3-one, 17-(1-oxobutoxy)-, (5α,17β)-
RN: 18069-66-4 **MP** (°C)**:**
MW: 360.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.220E-06	4.400E-04	ns	B057	0 2 1 1 2	

4363. $C_{23}H_{38}O_3$
Hexadecyl *p*-hydroxybenzoate
Hexadecyl 4-hydroxybenzoate
RN: 71067-09-9 **MP** (°C)**:**
MW: 362.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-03	3.789E-01	25	D081	1 2 2 1 2	

4364. $C_{23}H_{40}O_5$

4-Nonylphenol tetraethoxylate
p-Nonylphenol tetraethoxylate
RN: 7311-27-5 **MP** (°C)**:**
MW: 396.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-05	7.650E-03	20.5	A335	0 0 0 0 0	
1.930E-05	7.654E-03	20.5	A335	0 0 0 0 0	

4365. $C_{24}H_{12}$

Coronene
Coronen
RN: 191-07-1 **MP** (°C)**:** 438
MW: 300.36 **BP** (°C)**:** 525

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-09	1.406E-06	20	E009	1 0 0 1 2	
3.329E-10	1.000E-07	25	B319	2 0 1 2 1	
4.661E-10	1.400E-07	25	M064	1 1 2 2 1	
4.660E-10	1.400E-07	25	M342	1 0 1 1 2	

4366. $C_{24}H_{20}N_2$

N,*N*′-Diphenylbenzidine
RN: 531-91-9 **MP** (°C)**:** 247
MW: 336.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-07	6.000E-05	50	K068	1 0 2 2 0	buffer
1.783E-07	6.000E-05	rt	K068	0 0 2 2 0	buffer

4367. $C_{24}H_{22}N_2O_2$

G-3
p-Phenylpropylphenylbutazone
3,5-Pyrazolidinedione, 1,2-diphenyl-4-(3-phenylpropyl)-
RN: 32060-78-9 **MP** (°C)**:**
MW: 370.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.779E-04	1.400E-01	ns	B158	0 0 0 0 1	pH 7.0

4368. $C_{24}H_{26}N_2O_4$
Carvedilol
RN: 72956-09-3 **MP** (°C)**:**
MW: 406.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.492E-04	22.5	B440	0 0 0 0 0	
7.380E-05	3.000E-02	ns	S469	0 0 0 0 0	

4369. $C_{24}H_{26}N_4O_2$
Methyldiantipyrylmethane
MDAM
RN: 1606-56-0 **MP** (°C)**:**
MW: 402.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-03	4.498E-01	20	P054	0 0 0 0 0	

4370. $C_{24}H_{26}N_4S_2$
Methyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-ethylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-70-5 **MP** (°C)**:** 229
MW: 434.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.173E-01	ns	D087	0 2 0 0 1	

4371. $C_{24}H_{27}BrN_6O_{10}$
C.I. Disperse blue 79
2′-Acetylamino-4′-[bis(acetoxyethyl)amino]-6-bromo-2,4-dinitro-5′-ethoxyazobenzene
RN: 12239-34-8 **MP** (°C)**:** 146
MW: 639.43 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-09	6.394E-07	25	B333	0 0 0 0 0	

4372. $C_{24}H_{27}N$
Prenylamine
N-(3,3-Diphenylpropyl)-α-methylphenylethylamine
RN: 390-64-7 **MP** (°C)**:** 36.5
MW: 329.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.517E-04	5.000E-02	37	C054	2 0 2 1 0	

4373. $C_{24}H_{29}N_5O_3$
Valsartan
(2*S*)-3-Methyl-2-[pentanoyl-[[4-[2-(2H-tetrazol-5-yl)phenyl]phenyl]methyl]amino]butanoic acid
RN: 137862-53-4 **MP** (°C)**:**
MW: 435.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.951E-04	8.499E-02	25	C431	0 0 0 0 0	

4374. $C_{24}H_{30}F_2O_6$
Fluocinolone acetonide
6α,9α-Difluoro-16α hydroxyprednisolone-16,17-acetonide
6α,9α-Difluoro-16α,17α-isopropylidenedioxy-1,4-pregnadiene-3,20-dione
RN: 67-73-2 **MP** (°C)**:** 260.5
MW: 452.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-04	1.080E-01	25	K021	1 2 2 2 1	
4.641E-05	2.100E-02	25	O001	2 0 2 2 2	
2.210E-04	1.000E-01	25	P008	0 0 0 0 0	EFG

4375. $C_{24}H_{31}ClO_7$
Loteprednol etabonate
Lenoxin
Androsta-1,4-diene-17-carboxylic acid
17-[(Ethoxycarbonyl)oxy]-11-hydroxy-3-oxo-chloromethyl ester, (11b,17a)-
RN: 82034-46-6 **MP** (°C)**:**
MW: 466.96 **BP** (°C)**:** 600.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.14E-06	<1.00E-03	23	B409	1 0 0 0 1	

4376. $C_{24}H_{31}FO_5S$
Timobesone acetate
17-β-Methythiocarbonyl-9α-fluoro-11β
RN: 79578-14-6 **MP** (°C)**:**
MW: 450.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	2.703E+00	25	O318	0 0 0 0 0	

4377. $C_{24}H_{31}FO_6$

Triamcinolone acetonide
9α-Fluoro-16α-hydroxyprednisolone acetonide
Triamcinolone 16α,17-acetonide
Aristoderm
Adcortyl-A

RN: 76-25-5 **MP** (°C)**:** 293
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.205E-05	4.000E-02	23	F025	1 0 0 0 0	
9.436E-05	4.100E-02	25	K021	1 2 2 2 1	
6.076E-04	2.640E-01	25	L009	1 0 0 1 1	
4.833E-05	2.100E-02	28	B055	2 0 2 2 2	
4.027E-05	1.750E-02	28	B056	1 2 1 1 2	
5.869E-05	2.550E-02	37	B055	2 0 2 2 2	
4.764E-05	2.070E-02	37	B056	1 2 1 1 2	
9.205E-05	4.000E-02	37	F025	1 0 0 0 0	
7.733E-05	3.360E-02	50	B055	2 0 2 2 2	
6.099E-05	2.650E-02	50	B056	1 2 1 1 2	
2.532E-04	1.100E-01	amb	L434	0 0 0 0 0	

4378. $C_{24}H_{31}FO_6$

Betamethasone acetate
Betamethasone-17-acetate
9α-Fluoro-16β-methylprednisolone-21-acetate

RN: 987-24-6 **MP** (°C)**:** 200dec
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.904E-05	3.000E-02	25	K003	2 1 1 1 1	

4379. $C_{24}H_{31}FO_6$

Dexamethasone acetate
Dexamethasone-17-acetate
Dexamethasone acetate

RN: 1177-87-3 **MP** (°C)**:** 263
MW: 434.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.992E-05	1.300E-02	25	K003	2 1 1 1 1	
6.214E-05	2.700E-02	37	D026	0 0 0 0 0	

4380. $C_{24}H_{31}NO_4$

Drotaverine
1-(3,4-Diethoxybenzylidene)-6,7-diethoxy-1,2,3,4-tetrahydroisoquinoline
RN: 14009-24-6 **MP** (°C)**:**
MW: 397.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-02	1.375E+01	37	C054	2 0 2 1 2	

4381. $C_{24}H_{32}N_2O_9$

Enalapril maleate
L-Proline, 1-[*N*-[1-(ethoxycarbonyl)-3-phenylpropyl]-L-alanyl]-,
(*S*)-1-(*N*-(1-(Ethoxycarbonyl)-3-phenylpropyl)-L-alanyl)-L-proline, (Z)-2-butenedioate salt
RN: 76095-16-4 **MP** (°C)**:**
MW: 492.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.264E-02	2.100E+01	25	A412	1 0 2 2 1	int

4382. $C_{24}H_{32}O_4$

Ethynodiol diacetate
Ovulen-50
RN: 297-76-7 **MP** (°C)**:** 126
MW: 384.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.641E-06	1.400E-03	25	L027	1 0 0 0 2	

4383. $C_{24}H_{32}O_4S$

Spironolactone
17-Hydroxy-7α-mercapto-3-oxo-17α-pregn-4-ene-21-carboxylic acid γ-lactone acetate
Spiractin
RN: 52-01-7 **MP** (°C)**:** 134
MW: 416.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-06	2.999E-03	25	A348	0 0 0 0 0	
5.281E-05	2.200E-02	25	C037	2 1 2 2 2	
5.281E-05	2.200E-02	25	G084	2 0 2 2 1	
4.801E-05	2.000E-02	25	G095	2 1 2 2 1	
6.649E-05	2.770E-02	37	K092	2 0 0 1 2	
2.400E-05	1.000E-02	ns	K444	0 0 0 0 0	

4384. $C_{24}H_{32}O_5$
7-Carboxylic acid methyl ester canrenone
RN: **MP** (°C)**:**
MW: 400.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	7.850E-02	37	C004	0 0 0 0 0	EFG

4385. $C_{24}H_{32}O_6$
Cortisone 17-propionate
Pregn-4-ene-3,11,20-trione, 21-hydroxy-17-(1-oxopropoxy)-
RN: 136370-32-6 **MP** (°C)**:**
MW: 416.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.921E-05	8.000E-03	25	M023	1 0 2 1 0	

4386. $C_{24}H_{33}FO_6$
Flurandrenolone
Fludroxycortide
6-Fluoro-16α-hydroxyhydrocortisone-16,17-acetonide
RN: 1524-88-5 **MP** (°C)**:**
MW: 436.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.758E-04	2.950E-01	25	K021	1 2 2 2 1	

4387. $C_{24}H_{34}N_2O$
Bepridil
1-Isobutoxy-2-pyrrolidino-3-*N*-benzylanilino-propane
Bepadin
RN: 64706-54-3 **MP** (°C)**:**
MW: 366.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.027E-02	7.430E+00	37	N032	1 0 1 1 2	

4388. $C_{24}H_{34}N_2O_3$
Lysine estrone ester
RN: **MP** (°C)**:**
MW: 398.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	1.260E+02	ns	A074	0 0 0 0 0	EFG

4389. $C_{24}H_{34}O_5$

Dehydrocholic acid
3,7,12-Trioxo-5β-cholanic acid
RN: 81-23-2 **MP** (°C)**:** 237
MW: 402.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-04	1.800E-01	15	G081	1 0 1 1 1	
1.615E-04	6.500E-02	30	O321	0 0 0 0 0	
1.600E-04	6.441E-02	30	O321	0 0 0 0 0	

4390. $C_{24}H_{34}O_6$

Hydrocortisone propionate
Hydrocortisone-21-propionate
RN: 6677-98-1 **MP** (°C)**:**
MW: 418.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.772E-05	1.160E-02	25	H098	1 0 2 0 2	
2.772E-05	1.160E-02	25	H320	0 0 0 0 0	
2.770E-05	1.159E-02	25	H320	0 0 0 0 0	

4391. $C_{24}H_{36}O_3$

Testosterone valerate
Androst-4-en-3-one, 17-[(1-oxopentyl)oxy]-, (17β)-
Testosterone 17-valerate
RN: 3129-43-9 **MP** (°C)**:**
MW: 372.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.778E-07	2.898E-04	25	J004	1 0 1 1 2	
7.811E-07	2.910E-04	ns	B057	0 2 1 1 2	

4392. $C_{24}H_{36}O_3$

5,6-Dehydroisoandrosterone valerate
Androst-5-en-17-one, 3-[(1-oxopentyl)oxy]-, (3β)-
RN: 7642-68-4 **MP** (°C)**:**
MW: 372.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.061E-05	7.680E-03	ns	B057	0 2 1 1 2	

4393. $C_{24}H_{38}O_3$
Androstanolone valerate
Androstan-3-one, 17-[(1-oxopentyl)oxy]-, (5α,17β)-
RN: 26271-72-7 **MP** (°C)**:**
MW: 374.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.143E-07	3.050E-04	ns	B057	0 2 1 1 2	

4394. $C_{24}H_{38}O_4$
Di-2-ethylhexyl isophthalate
D-(2-Ethylhexyl) isophthalate
Dioctyl isophthalate
RN: 137-89-3 **MP** (°C)**:**
MW: 390.57 **BP** (°C)**:** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.816E-08	1.100E-05	24	H116	2 1 0 0 2	

4395. $C_{24}H_{38}O_4$
Octyl phthalate
Di(2-ethylhexyl)phthalate
Di-(2-ethylhexyl)-phthalate
Di-*sec*-octyl phthalate
bis(2-Ethylhexyl) phthalate
bis-(2-Ethylhexyl) 1,2-benzenedicarboxylate
RN: 117-81-7 **MP** (°C)**:** –50
MW: 390.57 **BP** (°C)**:** 386.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	9.999E-02	20	F070	1 0 0 0 1	*sic*
1.050E-07	4.101E-05	20	L300	2 1 0 2 2	
1.536E-06	6.000E-04	22.5	G301	0 0 0 0 0	
7.297E-07	2.850E-04	24	H116	2 1 0 0 2	
6.913E-07	2.700E-04	25	D336	0 0 0 0 0	
1.280E-06	5.000E-04	25	F067	1 0 2 2 0	

4396. $C_{24}H_{38}O_4$
Apocholic acid
RN: 641-81-6 **MP** (°C)**:** 175.5
MW: 390.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-03	8.000E-01	15	G081	1 0 1 1 0	

4397. $C_{24}H_{38}O_4$
bis(Tereoctyl) phthalate
RN: **MP** (°C)**:**
MW: 390.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.633E-08	2.200E-05	25	D336	0 0 0 0 0	

4398. $C_{24}H_{38}O_4$
bis(Isooctyl) phthalate
Diisooctyl phthalate
1,2-Benzenedicarboxylic acid diisooctyl ester
RN: 27554-26-3 **MP** (°C)**:** -4
MW: 390.57 **BP** (°C)**:** 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E-07	4.000E-05	25	D336	0 0 0 0 0	

4399. $C_{24}H_{38}O_4$
bis(*n*-Octyl) phthalate
Di-*n*-octyl phthalate
1,2-Benzenedicarboxylic acid
RN: 117-84-0 **MP** (°C)**:** –25
MW: 390.57 **BP** (°C)**:** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-08	2.000E-05	25	D336	0 0 0 0 0	

4400. $C_{24}H_{39}NO_3$
Acetaminophen palmitate
Acetaminophen hexadecanoate
RN: 54942-40-4 **MP** (°C)**:** 117
MW: 389.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.283E-05	5.000E-03	25	B010	1 1 1 1 0	

4401. $C_{24}H_{40}N_8O_4$
Dypyridamole
2,6-bis(Diethanolamino)-4,8-dipiperidinopyrimido-[5,4-d]pyrimidin
Dipridacot
Dipryridamole
Persantin
Dipyridamol
RN: 58-32-2 **MP** (°C)**:**
MW: 504.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.649E-06	8.320E-04	22.5	B440	0 0 0 0 0	
7.000E-05	3.532E-02	30	A417	0 0 0 0 0	pH 5.2
3.200E-03	1.615E+00	30	A417	0 0 0 0 0	pH 3.7

4402. $C_{24}H_{40}O_3$
3β-Hydroxy-5β-cholanoic acid
7α-Hydroxy-5β-cholanoic acid
RN: **MP** (°C)**:**
MW: 376.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	6.779E-05	10	F307	1 2 2 2 2	pH 3.0
4.400E-07	1.657E-04	10	F307	1 2 2 2 2	pH 3.0
5.200E-07	1.958E-04	15	F307	1 2 2 2 2	pH 3.0
2.200E-07	8.285E-05	15	F307	1 2 2 2 2	pH 3.0
2.400E-07	9.038E-05	20	F307	1 2 2 2 2	pH 3.0
6.500E-07	2.448E-04	20	F307	1 2 2 2 2	pH 3.0
2.800E-07	1.054E-04	25	F307	1 2 2 2 2	pH 3.0
7.900E-07	2.975E-04	25	F307	1 2 2 2 2	pH 3.0
3.500E-07	1.318E-04	30	F307	1 2 2 2 2	pH 3.0
9.700E-07	3.653E-04	30	F307	1 2 2 2 2	pH 3.0
5.300E-07	1.996E-04	35	F307	1 2 2 2 2	pH 3.0
1.190E-06	4.481E-04	35	F307	1 2 2 2 2	pH 3.0
8.200E-07	3.088E-04	40	F307	1 2 2 2 2	pH 3.0
1.490E-06	5.611E-04	40	F307	1 2 2 2 2	pH 3.0
1.770E-06	6.666E-04	45	F307	1 2 2 2 2	pH 3.0
1.280E-06	4.820E-04	45	F307	1 2 2 2 2	pH 3.0
1.500E-06	5.649E-04	50	F307	1 2 2 2 2	pH 3.0
2.150E-06	8.097E-04	50	F307	1 2 2 2 2	pH 3.0

4403. $C_{24}H_{40}O_3$

Lithocholic acid
3α-Hydroxy-5β-cholan-24-oic acid
3α-Hydroxycholanic acid
RN: 434-13-9 **MP** (°C)**:** 184
MW: 376.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.431E-05	10	F307	1 2 2 2 2	pH 3.0
4.000E-08	1.506E-05	15	F307	1 2 2 2 2	pH 3.0
4.600E-08	1.732E-05	20	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	20	I012	1 2 2 1 0	pH 2.4
5.000E-08	1.883E-05	25	F307	1 2 2 2 2	pH 3.0
6.000E-08	2.260E-05	30	F307	1 2 2 2 2	pH 3.0
7.500E-08	2.824E-05	35	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	37	I012	1 2 2 1 0	pH 2.4
1.000E-07	3.766E-05	40	F307	1 2 2 2 2	pH 3.0
1.100E-07	4.142E-05	45	F307	1 2 2 2 2	pH 3.0
1.400E-07	5.272E-05	50	F307	1 2 2 2 2	pH 3.0

4404. $C_{24}H_{40}O_4$

Hyodeoxycholic acid
3α,6β-Dihydroxy-5α-cholanoic acid
RN: 83-49-8 **MP** (°C)**:** 198
MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.926E-03	10	F307	1 2 2 2 2	pH 3.0
1.200E-05	4.711E-03	15	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	20	F307	1 2 2 2 2	pH 3.0
1.500E-05	5.889E-03	25	F307	1 2 2 2 2	pH 3.0
1.700E-05	6.674E-03	30	F307	1 2 2 2 2	pH 3.0
1.800E-05	7.067E-03	35	F307	1 2 2 2 2	pH 3.0
2.000E-05	7.852E-03	40	F307	1 2 2 2 2	pH 3.0
2.200E-05	8.637E-03	45	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	50	F307	1 2 2 2 2	pH 3.0

4405. $C_{24}H_{40}O_4$

Deoxycholic acid
Cholan-24-oic acid, 3,12-dihydroxy-, (3α,5β,12α)-
3α,12α-Dihydroxy-5β-cholanoic acid
RN: 83-44-3 **MP** (°C)**:** 176
MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-05	9.422E-03	10	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	15	F307	1 2 2 2 2	pH 3.0
6.113E-04	2.400E-01	15	G081	1 0 1 1 1	

(*continued*)

4405. $C_{24}H_{40}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.093E-04	2.000E-01	20	D041	1 0 0 0 0	
2.700E-05	1.060E-02	20	F307	1 2 2 2 2	pH 3.0
1.110E-04	4.358E-02	20	I012	1 2 2 1 2	pH 2.4
2.800E-05	1.099E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
2.900E-05	1.138E-02	35	F307	1 2 2 2 2	pH 3.0
1.140E-04	4.475E-02	37	I012	1 2 2 1 2	pH 2.4
2.900E-05	1.138E-02	40	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	45	F307	1 2 2 2 2	pH 3.0
3.200E-05	1.256E-02	50	F307	1 2 2 2 2	pH 3.0

4406. $C_{24}H_{40}O_4$

Chenodeoxycholic acid

CDCA

RN: 474-25-9 **MP** (°C)**:** 119

MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	9.815E-03	10	F307	1 2 2 2 2	pH 3.0
2.500E-05	9.815E-03	15	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	20	F307	1 2 2 2 2	pH 3.0
2.290E-04	8.990E-02	20	I012	1 2 2 1 2	pH 2.4
2.700E-05	1.060E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	35	F307	1 2 2 2 2	pH 3.0
2.560E-04	1.005E-01	37	I008	1 0 0 1 2	
2.560E-04	1.005E-01	37	I012	1 2 2 1 2	pH 2.4
3.150E-05	1.237E-02	40	F307	1 2 2 2 2	pH 3.0
3.400E-05	1.335E-02	45	F307	1 2 2 2 2	pH 3.0
3.600E-05	1.413E-02	50	F307	1 2 2 2 2	pH 3.0
2.291E-04	8.994E-02	ns	R427	0 0 0 0 0	

4407. $C_{24}H_{40}O_4$

Ursodeoxycholic acid

UDCA

RN: 128-13-2 **MP** (°C)**:** 203

MW: 392.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.748E-03	10	F307	1 2 2 2 2	pH 3.0
7.500E-06	2.944E-03	15	F307	1 2 2 2 2	pH 3.0
8.000E-06	3.141E-03	20	F307	1 2 2 2 2	pH 3.0
5.100E-05	2.002E-02	20	I012	1 2 2 1 1	pH 2.4
9.000E-06	3.533E-03	25	F307	1 2 2 2 2	pH 3.0
1.000E-05	3.926E-03	30	F307	1 2 2 2 2	pH 3.0

(*continued*)

4407. $C_{24}H_{40}O_4$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-05	4.515E-03	35	F307	1 2 2 2 2	pH 3.0
5.300E-05	2.081E-02	37	I008	1 0 0 1 1	
5.300E-05	2.081E-02	37	I012	1 2 2 1 1	pH 2.4
1.200E-05	4.711E-03	40	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	45	F307	1 2 2 2 2	pH 3.0
1.400E-05	5.496E-03	50	F307	1 2 2 2 2	pH 3.0
8.556E-04	3.359E-01	ns	K446	0 0 0 0 0	

4408. $C_{24}H_{40}O_5$

3α, 6α, 7α -Trihydroxy-5β-cholanate

RN: **MP** (°C)**:**

MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-05	1.512E-02	10	F307	1 2 2 2 2	pH 3.0
3.800E-05	1.553E-02	15	F307	1 2 2 2 2	pH 3.0
4.100E-05	1.675E-02	20	F307	1 2 2 2 2	pH 3.0
4.500E-05	1.839E-02	25	F307	1 2 2 2 2	pH 3.0
5.500E-05	2.247E-02	30	F307	1 2 2 2 2	pH 3.0
6.900E-05	2.819E-02	35	F307	1 2 2 2 2	pH 3.0
8.600E-05	3.514E-02	40	F307	1 2 2 2 2	pH 3.0
1.160E-04	4.740E-02	45	F307	1 2 2 2 2	pH 3.0
1.600E-04	6.537E-02	50	F307	1 2 2 2 2	pH 3.0

4409. $C_{24}H_{40}O_5$

Ursocholic acid

3α,7β,12α-Trihydroxy-5β-cholanoic acid

RN: 2955-27-3 **MP** (°C)**:**

MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-03	6.496E-01	10	F307	1 2 2 2 2	pH 3.0
1.610E-03	6.578E-01	15	F307	1 2 2 2 2	pH 3.0
1.640E-03	6.701E-01	20	F307	1 2 2 2 2	pH 3.0
1.670E-03	6.823E-01	25	F307	1 2 2 2 2	pH 3.0
1.710E-03	6.987E-01	30	F307	1 2 2 2 2	pH 3.0
1.762E-03	7.199E-01	35	F307	1 2 2 2 2	pH 3.0
1.828E-03	7.469E-01	40	F307	1 2 2 2 2	pH 3.0
1.872E-03	7.649E-01	45	F307	1 2 2 2 2	pH 3.0
2.000E-03	8.172E-01	50	F307	1 2 2 2 2	pH 3.0

4410. $C_{24}H_{40}O_5$
Cholic acid
Cholsaeure
RN: 81-25-4 **MP** (°C)**:** 198
MW: 408.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-04	9.030E-02	10	F307	1 2 2 2 2	pH 3.0
6.486E-04	2.650E-01	15	F300	1 0 0 0 0	
2.140E-04	8.744E-02	15	F307	1 2 2 2 2	pH 3.0
6.853E-04	2.800E-01	15	G081	1 0 1 1 1	
6.851E-04	2.799E-01	20	D041	1 0 0 0 1	
2.247E-04	9.180E-02	20	E008	1 0 2 0 2	average of 3
2.200E-04	8.989E-02	20	F307	1 2 2 2 2	pH 3.0
4.280E-04	1.749E-01	20	I012	1 2 2 1 2	pH 2.4
2.350E-04	9.602E-02	25	F307	1 2 2 2 2	pH 3.0
2.670E-04	1.091E-01	30	F307	1 2 2 2 2	pH 3.0
3.240E-04	1.324E-01	35	F307	1 2 2 2 2	pH 3.0
4.600E-04	1.879E-01	37	I012	1 2 2 1 2	pH 2.4
3.830E-04	1.565E-01	40	F307	1 2 2 2 2	pH 3.0
4.830E-04	1.973E-01	45	F307	1 2 2 2 2	pH 3.0
6.390E-04	2.611E-01	50	F307	1 2 2 2 2	pH 3.0

4411. $C_{24}H_{50}$
Tetracosane
n-Tetracosane
Alkane C(24)
RN: 646-31-1 **MP** (°C)**:** 54
MW: 338.67 **BP** (°C)**:** 391.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.264E-02	4.282E+00	321	S355	1 1 1 2 0	EFG
8.878E-02	3.007E+01	369	S355	1 1 1 2 0	EFG

4412. $C_{24}H_{51}OP$
tri-*n*-Octylphosphine oxide
TOPO
Trioctylphosphine oxide
RN: 78-50-2 **MP** (°C)**:**
MW: 386.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-06	2.800E-03	0	O002	2 0 2 2 1	
3.880E-06	1.500E-03	25	O002	2 0 2 2 1	

4413. $C_{24}H_{51}O_3P$
Dibutyl hexadecyl phosphonate
Phosphonic acid, hexadecyl-, dibutyl ester
RN: 84869-93-2 **MP** (°C)**:**
MW: 418.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.78E-04	<2.00E-01	25	B070	1 2 0 1 0	

4414. $C_{24}H_{51}O_4P$
tris-(2-Ethylhexyl) phosphate
Disflamoll TOF
TEHP
Flexol TOF
RN: 78-42-2 **MP** (°C)**:**
MW: 434.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-06	6.000E-04	24	H116	2 1 0 0 2	

4415. $C_{24}H_{54}OSn_2$
bis(Tributyltin) oxide
6-Oxa-5,7-distannaundecane, 5,5,7,7-tetrabutyl-
RN: 56-35-9 **MP** (°C)**:**
MW: 596.08 **BP** (°C)**:** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E-04	1.000E-01	rt	M161	0 0 0 0 2	

4416. $C_{25}H_{22}O_{10}$
Silybin
Silibinin
Silybum substance E6
Silymarin I
RN: 22888-70-6 **MP** (°C)**:**
MW: 482.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.788E-05	4.240E-02	19.99	B439	0 0 0 0 0	
1.119E-04	5.400E-02	24.99	B439	0 0 0 0 0	
1.432E-04	6.910E-02	29.99	B439	0 0 0 0 0	
1.726E-04	8.329E-02	34.99	B439	0 0 0 0 0	
2.066E-04	9.969E-02	39.99	B439	0 0 0 0 0	

4417. $C_{25}H_{24}F_6N_4$
Hydramethylnon
Amdro
Comat
Amidinohydrazone;
Wipeout
Tetrahydro-5,5-dimethyl-2(1H)-pyrimidinone[3-[4-(trifluoromethyl)phenyl]-1-[2-[4-(trifluoromethyl)phenyl]ethenyl]-2-propenylidene]hydrazone
RN: 67485-29-4 **MP** (°C)**:** 185–190
MW: 494.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-08	5.945E-06	ns	R427	0 0 0 0 0	

4418. $C_{25}H_{24}N_2O_2S$
G-8
o,p-Dimethylphenylthioethylphenylbutazone
3,5-Pyrazolidinedione, 1,2-diphenyl-4-[2-(2,4-xylylthio)ethyl]-
RN: 102892-46-6 **MP** (°C)**:**
MW: 416.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-04	1.300E-01	ns	B158	0 0 0 0 1	pH 7.0

4419. $C_{25}H_{28}N_4O_2$
Ethyldiantipyrylmethane
EDAM
RN: 61358-28-9 **MP** (°C)**:**
MW: 416.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.601E-04	1.500E-01	20	P054	0 0 0 0 0	

4420. $C_{25}H_{28}O_3$
Estradiol benzoate
Estradiol monobenzoate
7β-Estradiol-3-benzoate
RN: 50-50-0 **MP** (°C)**:** 190
MW: 376.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-06	4.000E-04	25	K003	2 1 1 1 1	
1.072E-06	4.034E-04	ns	R427	0 0 0 0 0	

4421. $C_{25}H_{28}O_3$
Ethofenprox
1-((2-(4-Ethoxyphenyl)-2-methylpropoxy)methyl)-3-phenoxybenzene
Etofenprox
Zoecon
MTI-500
Trebon
RN: 80844-07-1 **MP** (°C)**:**
MW: 376.50 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-09	9.457E-07	ns	R427	0 0 0 0 0	

4422. $C_{25}H_{29}I_2NO_3$
Amiodarone
Cordarone
Aratac
RN: 1951-25-3 **MP** (°C)**:**
MW: 645.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.72E-08	<4.34E-05	22.5	B440	0 0 0 0 0	
1.110E-03	7.164E-01	25	B337	2 2 2 1 2	

4423. $C_{25}H_{31}FO_8$
Triamcinolone 16, 21-diacetate
Pregna-1,4-diene-3,20-dione, 16,21-bis(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β,16apha)-
RN: 67-78-7 **MP** (°C)**:** 235
MW: 478.52 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-04	4.800E-02	25	F026	0 0 0 0 0	

4424. $C_{25}H_{31}NO_2$
3-Hydroxy-17β-{[(1-methyl-1,4-dihydropyridin-3-yl)-carbonyl]oxy}-estra-1,3,5(10)-triene
RN: **MP** (°C)**:**
MW: 377.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-07	6.580E-05	25	B366	0 0 0 0 0	

4425. $C_{25}H_{34}O_3$
Norethindrone dimethylpropionate
19-Norpregn-4-en-20-yn-3-one, 17-(2,2-dimethyl-1-oxopropoxy)-, (17α)-
RN: 65445-09-2 **MP** (°C)**:**
MW: 382.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.894E-08	3.020E-05	25	L078	1 0 1 2 2	

4426. $C_{25}H_{34}O_6$
Budesonide
16,17-Butylidenebis(oxy)-11-,21-dihydroxypregna-1,4-diene-3,20-dione
Rhinocort
RN: 51333-22-3 **MP** (°C)**:**
MW: 430.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	2.153E-02	ns	F327	0 0 1 2 2	

4427. $C_{25}H_{34}O_9$
6-(1,3-Dihydro-7-acetate-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic solketal ester
RN: **MP** (°C)**:**
MW: 478.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-05	9.000E-03	25	L333	1 1 1 1 0	

4428. $C_{25}H_{35}N_5O_4$
Benzoic acid, 3-[(dibutylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c] pyridin-1-yl)methoxy]ethyl ester
1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.
RN: 137605-73-3 **MP** (°C)**:**
MW: 469.59 **BP** (°C)**:** 688.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-05	6.000E-03	21	B419	1 1 2 2 1	int

4429. $C_{25}H_{36}N_4O_7$
Nonyloxycarbonyl-mitomycin C
2′-(2-Hexanoyl-2-pentanyl-acetyl)-6-methoxypurine arabinoside
RN: **MP** (°C)**:**
MW: 504.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	1.261E-04	25	M316	1 1 1 1 2	
2.020E-03	1.019E+00	37	C348	0 0 0 0 0	pH 7.00

4430. $C_{25}H_{36}O_6$
Hydrocortisone butyrate
Hydrocortisone-21-butyrate
11,17-Dihydroxy-21-(1-oxobutoxy)-pregn-4-ene-3,20-dione
RN: 6677-99-2 **MP** (°C)**:**
MW: 432.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-05	7.730E-03	25	H098	1 0 2 0 2	
1.787E-05	7.730E-03	25	H320	0 0 0 0 0	
1.780E-05	7.700E-03	25	H320	0 0 0 0 0	

4431. $C_{25}H_{36}O_7$
5,16-β-Dihydroxy-6-β-methyl-3,11-dioxo-5-α-pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester cycl
RN: **MP** (°C)**:**
MW: 448.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.672E-04	7.500E-02	ns	K029	0 0 2 1 1	

4432. $C_{25}H_{40}O_3Si_2$
Norethindrone pentamethyldisiloxyl ether
RN: **MP** (°C)**:**
MW: 444.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.301E-07	1.023E-04	25	L078	1 0 1 2 2	

4433. $C_{25}H_{42}O_3$
Octadecyl-*p*-hydroxybenzoate
RN: 71067-10-2 **MP** (°C)**:**
MW: 390.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.343E-04	3.259E-01	25	D081	1 2 2 1 2	

4434. $C_{25}H_{44}$
Nonadecylbenzene
1-Phenylnonadecane
RN: 29136-19-4 **MP** (°C)**:**
MW: 344.63 **BP** (°C)**:** 419

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-02	5.272E+00	328	S355	1 1 1 2 0	EFG
2.396E-01	8.257E+01	363	S355	1 1 1 2 0	EFG

4435. $C_{25}H_{44}O_6$
4-Nonylphenol pentaethoxylate
RN: 20636-48-0 **MP** (°C)**:**
MW: 440.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E-05	9.480E-03	20.5	A335	0 0 0 0 0	
2.150E-05	9.473E-03	20.5	A335	0 0 0 0 0	

4436. $C_{25}H_{48}O_4$
Dioctyl azelate
Di(2-ethylhexyl) azelate
RN: 103-24-2 **MP** (°C)**:**
MW: 412.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.423E-07	1.000E-04	25	F067	1 0 2 2 0	

4437. $C_{25}H_{54}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)methane
HDPM
RN: 2785-33-3 **MP** (°C)**:**
MW: 448.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	6.400E-02	0	O002	2 0 2 2 0	EFG
8.849E-05	3.970E-02	25	O002	2 0 2 2 1	average of 2
6.241E-05	2.800E-02	35	O002	2 0 2 2 0	EFG
4.458E-05	2.000E-02	40	O002	2 0 2 2 0	EFG
3.377E-03	1.515E+00	45	O002	2 0 2 2 0	EFG

4438. $C_{26}H_{18}N_2O_4$
Samaron violet
Mowilith red 3B(IG)
RN: 6408-72-6 **MP** (°C)**:**
MW: 422.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	1.267E-03	98.59	M180	0 0 2 2 0	EFG
4.000E-06	1.690E-03	109.98	M180	0 0 2 1 0	EFG
4.500E-06	1.901E-03	120.54	M180	0 0 2 2 0	EFG
6.000E-06	2.535E-03	133.34	M180	0 0 2 2 0	EFG
8.000E-06	3.380E-03	141.78	M180	0 0 2 2 0	EFG

4439. $C_{26}H_{20}N_2O_8S_2$
1,5-Anthraquinone disulfonic acid anilide
RN: **MP** (°C)**:**
MW: 552.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.210E-03	3.984E+00	18	F047	1 2 1 1 1	

4440. $C_{26}H_{20}N_2O_8S_2$
1,8-Anthraquinone disulfonic acid anilide
RN: **MP** (°C)**:**
MW: 552.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.209E-02	2.326E+01	18	F047	1 2 1 1 1	

4441. $C_{26}H_{28}Cl_2N_4O_4$
Ketoconazole
(±)-*cis*-1-Acetyl-4-(4-[(2-[2,4-dichlorophenyl]-2-[1H-imidazol-1-ylmethyl]-1,3-dioxolan-4-yl)-methoxy]phenyl)piperazine
RN: 65277-42-1 **MP** (°C)**:**
MW: 531.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.505E-04	8.000E-02	37	C323	0 0 0 0 0	EFG
1.882E-05	1.000E-02	amb	L434	0 0 0 0 0	

4442. $C_{26}H_{28}N_2$
Cinnarizine
Stugeron
RN: 298-57-7 **MP** (°C)**:**
MW: 368.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.035E-03	7.500E-01	ns	B155	0 0 1 1 0	EFG, pH 3.0

4443. $C_{26}H_{28}N_4O_2$
Propyldiantipyrylmethane
PDAM
RN: 1461-17-2 **MP** (°C)**:**
MW: 428.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	6.000E-02	20	P054	0 0 0 0 0	

4444. $C_{26}H_{29}NO$
Tamoxifen
Genox
Kessar
Nolvadex
(Z)-2-[4-(1,2-Diphenyl-1-butenyl)phenoxy]-*N*,*N*-dimethylethanamine
Tamoxen
RN: 10540-29-1 **MP** (°C)**:**
MW: 371.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.550E+00	2.805E+03	25	B443	0 0 0 0 0	extrapolated
		amb	L434	0 0 0 0 0	

4445. $C_{26}H_{30}Cl_2F_3NO$

Halofantrine
1-(1,3-Dichloro-6-trifluoromethyl-9-phenanthryl)-3-di(*n*-butyl)aminopropanol
RN: 69756-53-2 **MP** (°C)**:**
MW: 500.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-06	5.900E-04	37	A423	0 0 0 0 0	

4446. $C_{26}H_{30}N_4O_2$

Isopropyldiantipyrylmethane
IPDAM
RN: 15536-49-9 **MP** (°C)**:**
MW: 430.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-04	2.000E-01	20	P054	0 0 0 0 0	

4447. $C_{26}H_{30}N_4S_2$

Propyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-butylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 57094-83-4 **MP** (°C)**:** 222
MW: 462.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	1.110E-01	ns	D087	0 2 0 0 1	

4448. $C_{26}H_{31}ClN_2O_8S$

Amlodipine
Amlodipine besylate
Norvasc
(*RS*)-3-Ethyl-5-methyl-2-(2-aminoethoxymethyl)-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridinedicarboxylate benzenesulfonate
RN: 88150-42-9 **MP** (°C)**:**
MW: 567.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.76E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4449. $C_{26}H_{32}F_2O_7$
Diflorasone diacetate
U-34865
RN: 33564-31-7 **MP** (°C)**:**
MW: 494.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.314E-05	6.500E-03	25	F003	0 0 0 0 0	
1.254E-05	6.200E-03	37	F003	0 0 0 0 0	
2.629E-05	1.300E-02	50	F003	0 0 0 0 0	

4450. $C_{26}H_{32}F_2O_7$
Fluocinolide
Fluocinonide
Fluocinolone acetonide acetate
RN: 356-12-7 **MP** (°C)**:**
MW: 494.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-06	5.300E-04	25	O001	2 0 2 2 2	
2.022E-05	1.000E-02	25	P008	0 0 0 0 0	EFG

4451. $C_{26}H_{32}O_3$
Testosterone benzoate
Androst-4-en-3-one, 17-(benzoyloxy)-, (17β)-
RN: 2088-71-3 **MP** (°C)**:**
MW: 392.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.312E-05	1.300E-02	25	L342	1 0 1 1 2	

4452. $C_{26}H_{36}O_3$
Norethisterone heptanoate
RN: **MP** (°C)**:**
MW: 396.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.521E-07	6.030E-05	25	E301	1 0 1 1 2	

4453. $C_{26}H_{36}O_6$
Prednisolone 21-trimethylacetate
Prednisolone acetate
RN: 52-21-1 **MP** (°C)**:** 233
MW: 444.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-05	1.160E-02	25	C037	2 1 2 2 2	
6.298E-05	2.800E-02	25	K021	1 2 2 2 1	
2.699E-05	1.200E-02	ns	N302	0 2 1 2 1	

4454. $C_{26}H_{37}FO_5$
Dexamethasone TBA
RN: **MP** (°C)**:**
MW: 448.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.229E-05	1.000E-02	37	D026	0 0 0 0 0	

4455. $C_{26}H_{38}NO_8$
Glucosamine testosterone
17-β-(4-Androsten-3-one)-*N*-2-(2-desoxyglucosyl)
RN: **MP** (°C)**:** 185–190
MW: 492.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	6.560E-01	25	L009	1 0 0 1 1	

4456. $C_{26}H_{38}O_4$
Trimethylcyclohexyl phthalate
bis(*cis*-3,3,5-Trimethylcyclohexyl) phthalate
RN: 245652-81-7 **MP** (°C)**:** 93
MW: 414.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-07	1.200E-04	24	H116	2 1 0 0 2	

4457. $C_{26}H_{38}O_6$
Hydrocortisone valerate
Hydrocortisone-21-valerate
RN: 6678-00-8 **MP** (°C)**:**
MW: 446.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.830E-06	3.050E-03	25	H098	1 0 2 0 2	
6.830E-06	3.050E-03	25	H320	0 0 0 0 0	
6.780E-06	3.028E-03	25	H320	0 0 0 0 0	

4458. $C_{26}H_{39}NO_3S$
4-Pregnene-20-one-3-spiro-2′-(4′-ethoxycarbonyl-1′,3′-thiazolidine)
RN: **MP** (°C)**:** 131–135
MW: 445.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.81E-06	~1.70E-03	ns	B199	0 0 0 0 0	

4459. $C_{26}H_{43}NO_3$
Acetaminophen stearate
Acetaminophen octadecanoate
Stearoyl acetaminophen
Octadecanoic acid, 4-(acetylamino)phenyl ester
Acetanilide, 4′-hydroxy-, stearate (ester)
RN: 20675-22-3 **MP** (°C)**:** 117
MW: 417.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-05	5.000E-03	25	B010	1 1 1 1 0	
3.592E-05	1.500E-02	37	D029	0 0 0 0 0	

4460. $C_{26}H_{43}NO_6$
Glycocholic acid
Glycine, *N*-[(3α,5β,7α,12α)-3,7,12-trihydroxy-24-oxocholan-24-yl]-
RN: 475-31-0 **MP** (°C)**:** 130
MW: 465.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.085E-04	3.299E-01	20	E035	1 2 0 0 1	
2.188E-03	1.019E+00	60	E035	1 2 0 0 2	
5.035E-03	2.344E+00	80	E035	1 2 0 0 2	
1.810E-02	8.428E+00	100	E035	1 2 0 0 1	

4461. $C_{26}H_{50}O_4$

Dioctyl sebacate
Sebacic acid bis(2-ethylhexyl) ester
RN: 122-62-3 **MP** (°C)**:** –67
MW: 426.69 **BP** (°C)**:** 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-07	1.000E-04	25	F067	1 0 2 2 0	

4462. $C_{26}H_{56}O_2P_2$

bis(Di-*n*-hexyl-phosphinyl)ethane
HDPE
RN: 2785-34-4 **MP** (°C)**:**
MW: 462.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.300E-02	0	O002	2 0 2 2 1	EFG
6.484E-06	3.000E-03	25	O002	2 0 2 2 1	
6.484E-06	3.000E-03	60	O002	2 0 2 2 1	EFG

4463. $C_{27}H_{22}Cl_2N_4$

Clofazimine
Lamprene
N,5-bis(4-Chlorophenyl)-3,4-dihydro-3-((1-methylethyl)imino)-2-phenazinamine
3-(*p*-Chloroanilino)-10-(*p*-chlorophenyl)-2,10-dihydro-2-(isopropylimino)phenazine
RN: 2030-63-9 **MP** (°C)**:** 211
MW: 473.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.11E-06	<1.00E-03	ns	B404	0 2 1 1 0	
2.112E-05	1.000E-02	ns	K444	0 0 0 0 0	
2.000E-04	9.468E-02	ns	O322	0 0 0 0 0	EFG

4464. $C_{27}H_{29}NO_{11}$

Adriamycin
Adriblastin
RN: 23214-92-8 **MP** (°C)**:** 205
MW: 543.53 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.607E-02	1.961E+01	ns	I312	0 0 0 0 0	

4465. $C_{27}H_{30}O_3$
Norethindrone benzoate
RN: **MP** (°C)**:**
MW: 402.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.019E-08	8.128E-06	25	L078	1 0 1 2 2	

4466. $C_{27}H_{32}N_4O_2$
Butyldiantipyrylmethane
BDAM
RN: 61358-30-3 **MP** (°C)**:**
MW: 444.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.748E-05	3.000E-02	20	P054	0 0 0 0 0	

4467. $C_{27}H_{32}N_4O_2$
Isobutyldiantipyrylmethane
IBDAM
RN: 16671-34-4 **MP** (°C)**:**
MW: 444.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	6.000E-02	20	P054	0 0 0 0 0	

4468. $C_{27}H_{32}N_4S_2$
Isobutyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-(3-methylbutylidene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 73429-89-7 **MP** (°C)**:** 209
MW: 476.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	7.627E-02	ns	D087	0 2 0 0 1	

4469. $C_{27}H_{32}O_{14}$
Naringin
4H-1-Benzopyran-4-one, 7-[[2-*O*-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (*S*)-
RN: 10236-47-2 **MP** (°C)**:**
MW: 580.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.700E-01	6	P070	1 2 1 1 1	
8.613E-04	5.000E-01	20	P070	1 2 1 1 1	
1.361E-03	7.900E-01	35	P070	1 2 1 1 1	
3.376E-03	1.960E+00	45	P070	1 2 1 1 2	
1.233E-02	7.160E+00	55	P070	1 2 1 1 2	
7.271E-02	4.221E+01	65	P070	1 2 1 1 2	
1.864E-01	1.082E+02	75	P070	1 2 1 1 2	

4470. $C_{27}H_{33}N_3O_8$
Rolitetracycline
N-(1-Pyrrolidinylmethyl)tetracycline
Syntetrin
Tetraverin
Synotodecin
RN: 751-97-3 **MP** (°C)**:** 162dec
MW: 527.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.79E-02	>2.00E+01	21	M044	2 0 2 2 0	

4471. $C_{27}H_{34}O_3$
Testosterone phenylacetate
Androst-4-en-3-one, 17-[(phenylacetyl)oxy]-, (17β)-
RN: 5704-03-0 **MP** (°C)**:**
MW: 406.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-05	8.970E-03	25	L342	1 0 1 1 2	
2.188E-05	8.895E-03	ns	R427	0 0 0 0 0	

4472. $C_{27}H_{34}O_{10}$
Cortisone tricarballylate
RN: **MP** (°C)**:**
MW: 518.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	7.000E-02	25	M023	1 0 2 1 0	

4473. $C_{27}H_{36}N_2O_4$
Repaglinide
RN: 135062-02-1 **MP** (°C)**:**
MW: 452.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.988E-04	8.999E-02	25	M448	0 0 0 0 0	Intrinsic, EFG

4474. $C_{27}H_{38}N_2O_6$
p-Ureidophenyl prostaglandin E2
RN: **MP** (°C)**:**
MW: 486.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	1.363E-02	25	A066	1 0 1 1 1	

4475. $C_{27}H_{38}O_3$
Norethindrone heptanoate
RN: **MP** (°C)**:**
MW: 410.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	6.026E-05	25	L078	1 0 1 2 2	

4476. $C_{27}H_{40}N_2O_6$
p-Ureidophenyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 488.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-05	3.372E-02	25	A066	1 0 1 1 1	

4477. $C_{27}H_{40}O_6$
Hydrocortisone tebutate
Hydrocortisone-21-hexanoate
Hydrocortisone-21-caproate
RN: 508-96-3 **MP** (°C)**:** 168
MW: 460.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.083E-06	1.420E-03	25	H098	1 0 2 0 2	
3.083E-06	1.420E-03	25	H320	0 0 0 0 0	
3.060E-06	1.409E-03	25	H320	0 0 0 0 0	

4478. $C_{27}H_{42}Cl_2N_2O_6$
α-Chloramphenicol palmitate
β-Chloramphenicol palmitate
Chloramphenicol palmitate
RN: 530-43-8 **MP** (°C)**:** 359
MW: 561.55 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	6.177E-06	20	M006	2 2 1 2 1	
8.500E-08	4.773E-05	20	M006	2 2 1 2 1	
1.500E-08	8.423E-06	25	M006	2 2 1 2 1	
9.600E-08	5.391E-05	25	M006	2 2 1 2 1	
7.123E-06	4.000E-03	28	R004	0 0 0 0 0	
1.800E-08	1.011E-05	29	M006	2 2 1 2 1	
1.440E-07	8.086E-05	29	M006	2 2 1 2 2	
2.700E-08	1.516E-05	32	M006	2 2 1 2 1	
2.600E-07	1.460E-04	32	M006	2 2 1 2 2	
3.100E-08	1.741E-05	35	M006	2 2 1 2 1	
3.800E-07	2.134E-04	35	M006	2 2 1 2 2	

4479. $C_{27}H_{42}N_4O_7.0.3H_2O$
2′-(2-Heptanoyl-2-hexanyl-acetyl)-6-methoxypurine arabinoside (0.3 hydrate)
RN: 145913-52-6 **MP** (°C)**:**
MW: 540.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-04	1.615E-01	37	C348	0 0 0 0 0	pH 7.00

4480. $C_{27}H_{42}O_3$
Diosgenin
(25*R*)-Spirost-5-en-3β-ol
RN: 512-04-9 **MP** (°C)**:** 204
MW: 414.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-08	2.000E-05	25	L033	1 0 2 1 0	

4481. $C_{27}H_{42}O_3$
Nandrolone nonanoate
RN: **MP** (°C)**:**
MW: 414.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-06	9.260E-04	37	C026	0 0 0 0 0	

4482. $C_{27}H_{43}NO_8$
N-Methylglucamine testosterone
17-β-(4-Androsten-3-one)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 183–185
MW: 509.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.633E-05	4.400E-02	25	L009	1 0 0 1 1	

4483. $C_{27}H_{44}N_4O_6$
2′-Hexadecyl-6-methoxypurine arabinoside
RN: 145913-43-5 **MP** (°C)**:** 97–99
MW: 520.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	9.893E-03	37	C348	0 0 0 0 0	pH 7.00

4484. $C_{27}H_{44}O$
Vitamin D3
Cholecalciferol
Activated 7-dehydrocholesterol
Oleovitamin D3
RN: 67-97-0 **MP** (°C)**:** 85
MW: 384.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.30E-01	25	P312	0 0 0 0 0	

4485. $C_{27}H_{58}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)propane
HDPP
RN: 2896-56-2 **MP** (°C)**:**
MW: 476.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-04	1.300E-01	0	O002	2 0 2 2 0	EFG
1.154E-04	5.500E-02	15	O002	2 0 2 2 0	EFG
3.566E-05	1.700E-02	25	O002	2 0 2 2 0	

4486. $C_{28}H_{29}F_2N_3O$
Pimozide
2-Benzimidazolinone, 1-[1-[4,4-bis(*p*-fluorophenyl)butyl]-4-piperidyl]-
Orap
RN: 2062-78-4 **MP** (°C)**:**
MW: 461.56 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.900E-03	30	P044	0 0 0 0 0	

4487. $C_{28}H_{31}FN_4O$
Astemizole
1-((4-Fluorophenyl)-methyl)-*N*-(1-(2-(4-methoxyphenyl)ethyl)-4-piperidinyl)-1H-benzimidazol-2-amine
Hismanal
RN: 68844-77-9 **MP** (°C)**:**
MW: 458.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	3.210E-01	30	A417	0 0 0 0 0	pH 5.8
3.700E-03	1.697E+00	30	A417	0 0 0 0 0	pH 3.8

4488. $C_{28}H_{36}O_3$
Testosterone phenyl propionate
Androst-4-en-3-one, 17-(1-oxo-3-phenylpropoxy)-, (17β)-
RN: 1255-49-8 **MP** (°C)**:**
MW: 420.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.350E-06	2.250E-03	25	L342	1 0 1 1 2	

4489. $C_{28}H_{36}O_{15}$
Neohesperidin dihydrochalcone
1-Propanone, 1-[4-[[2-*O*-(6-deoxy-a-L-mannopyranosyl)-b-D-glucopyranosyl]oxy]-2,6-dihydroxyphenyl]-3-(3-hydroxy-4-methoxyphenyl)-
Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-(6-deoxy-a-L-mannopyranosyl)-, b-D-
Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-a-L-rhamnopyranosyl-
Neohesperidin DHC
NHDC
RN: 20702-77-6 **MP** (°C)**:**
MW: 612.59 **BP** (°C)**:** 927.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.530E-06	4.000E-03	rt	B417	0 0 1 2 1	

4490. $C_{28}H_{38}N_6O_{11}S$

Sildenafil citrate

1-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo [4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl] sulfonyl]-4-methylpiperazine citrate

Viagra

RN: 171599-83-0 **MP** (°C)**:**

MW: 666.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.231E-03	3.488E+00	ns	S469	0 0 0 0 0	

4491. $C_{28}H_{39}NO_6$

p-Acetamidophenyl prostaglandin E2

RN: **MP** (°C)**:**

MW: 485.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	2.622E-02	25	A066	1 0 1 1 1	

4492. $C_{28}H_{39}NO_6$

2-Oxo-5-indolinyl prostaglandin F2α

Prosta-5,13-dien-1-oic acid, 9,11,15-trihydroxy-, 2,3-dihydro-2-oxo-1H-indol-5-yl ester, (5Z,9α,11α,13E,15S)-

RN: 74973-22-1 **MP** (°C)**:**

MW: 485.63 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	2.914E-02	25	A066	1 0 1 1 1	

4493. $C_{28}H_{39}N_3O_6$

α-Semicarbazono-*p*-tolyl prostaglandin E2

RN: **MP** (°C)**:**

MW: 513.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	1.284E-03	25	A066	1 0 1 1 1	

4494. $C_{28}H_{40}FNO_{11}.H_2O$

Glucosamine 9-α-fluorohyfrocortisome (monohydrate)

21-(9-α-Fluoro-11α, 17α-dihydroxy-4-pregnen-3,20-dione)-*N*-2-(2-desoxyglucosyl) carbamate

RN: **MP** (°C)**:** 176-178

MW: 603.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.964E-04	3.600E-01	25	L009	1 0 0 1 1	

4495. $C_{28}H_{41}N_3O_6$
α-Semicarbazono-*p*-tolyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 515.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	8.250E-03	25	A066	1 0 1 1 1	

4496. $C_{28}H_{42}FNO_{11}.H_2O$
Glucamine 9-α-fluorohyfrocortisome (monohydrate)
RN: **MP** (°C)**:** 105–110
MW: 605.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.456E-03	2.699E+00	25	L009	1 0 0 1 1	

4497. $C_{28}H_{42}O_6$
Hydrocortisone heptanoate
Hydrocortisone-21-heptanoate
RN: **MP** (°C)**:**
MW: 474.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.082E-06	9.880E-04	25	H098	1 0 2 0 2	
2.082E-06	9.880E-04	25	H320	0 0 0 0 0	
2.060E-06	9.778E-04	25	H320	0 0 0 0 0	

4498. $C_{28}H_{44}O_3$
Nandrolone decanoate
Deca-durabolin
Norandrostenolone decanoate
RN: 360-70-3 **MP** (°C)**:**
MW: 428.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-06	6.640E-04	37	C026	0 0 0 0 0	

4499. $C_{28}H_{46}O_4$
Di-*n*-decyl phthalate
RN: 84-77-5 **MP** (°C)**:**
MW: 446.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.388E-07	3.300E-04	24	H116	2 1 0 0 2	

4500. $C_{28}H_{46}O_4$
Diisodecyl phthalate
RN: 26761-40-0 **MP** (°C)**:**
MW: 446.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.269E-07	2.800E-04	24	H116	2 1 0 0 2	

4501. $C_{28}H_{60}O_2P_2$
bis(Di-*n*-hexyl-phosphinyl)butane
HDPB
RN: 2785-35-5 **MP** (°C)**:**
MW: 490.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-04	1.780E-01	0	O002	2 0 2 2 0	EFG
1.284E-04	6.300E-02	15	O002	2 0 2 2 0	EFG
4.076E-05	2.000E-02	25	O002	2 0 2 2 0	

4502. $C_{29}H_{20}N_2O_4$
1,4-Dibenzoylaminoanthraquinone
Benzamide, *N*,*N*′-(9,10-dihydro-3-methyl-9,10-dioxo-1,8-anthracenediyl)bis
RN: 4627-15-0 **MP** (°C)**:**
MW: 460.49 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	1.013E-02	50	G077	1 0 0 0 1	

4503. $C_{29}H_{27}N_5O_4$
m-Nitrophenyldiantipyrylmethane
m-NPhDAM
RN: 1606-53-7 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.887E-05	3.000E-02	20	P054	0 0 0 0 0	

4504. $C_{29}H_{27}N_5O_4$
o-Nitrophenyldiantipyrylmethane
o-NPhDAM
RN: 14957-18-7 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4505. $C_{29}H_{27}N_5O_4$
p-Nitrophenyldiantipyrylmethane
p-NPhDAM
RN: 55774-19-1 **MP** (°C)**:**
MW: 509.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4506. $C_{29}H_{28}N_4O_2$
Phenyldiantipyrylmethane
PhDAM
RN: 1861-84-3 **MP** (°C)**:**
MW: 464.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.165E-04	2.399E-01	20	P054	0 0 0 0 0	

4507. $C_{29}H_{28}N_4O_3$
o-Hydroxylphenyldiantipyrylmethane
o-HPhDAM
RN: 1606-55-9 **MP** (°C)**:**
MW: 480.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.08E-05	<1.00E-02	20	P054	0 0 0 0 0	

4508. $C_{29}H_{28}N_4S_2$
Phenyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-(phenylmethylene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-68-1 **MP** (°C)**:** 160
MW: 496.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-05	2.086E-02	ns	D087	0 2 0 0 1	

4509. $C_{29}H_{32}O_{13}$
Etoposide
4′-Demethylepipodophyllotoxin ethylidene-β-D-glucoside
Vepesid
VP-16
RN: 33419-42-0 **MP** (°C)**:** 236–251
MW: 588.57 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-04	1.145E-01	25	S466	0 0 0 0 0	
3.398E-04	2.000E-01	ns	D347	0 0 0 0 0	
3.388E-04	1.994E-01	ns	R427	0 0 0 0 0	

4510. $C_{29}H_{35}NO_2$
Mifepristone
RU-486
RN: 84371-65-3 **MP** (°C)**:**
MW: 429.61 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.748E-04	22.5	B440	0 0 0 0 0	

4511. $C_{29}H_{36}N_4O_2$
Hexyldiantipyrylmethane
HDAM
RN: 7660-44-8 **MP** (°C)**:**
MW: 472.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.230E-05	1.999E-02	20	P054	0 0 0 0 0	
4.232E-05	2.000E-02	20	P054	0 0 0 0 0	

4512. $C_{29}H_{36}N_4S_2$
Hexyldithiopyrylmethane
3H-Pyrazole-3-thione, 4,4′-heptylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-
RN: 74713-69-2 **MP** (°C)**:** 169
MW: 504.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	2.070E-02	0	D087	0 2 0 0 1	

4513. $C_{29}H_{38}Cl_2N_2O_3$

3β-Hydroxy-13α-amino-13,17-seco-5α-androstan-17-oic-13,17-lactam-4-*N*,*N*-*bis*-(chloroethyl) amino phenyl-acetate

RN: **MP** (°C)**:**
MW: 533.54 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.186E-07	1.700E-04	25	P022	0 0 0 0 0	
3.599E-07	1.920E-04	30	P022	0 0 0 0 0	
4.517E-07	2.410E-04	44	P022	0 0 0 0 0	
6.110E-07	3.260E-04	73	P022	0 0 0 0 0	

4514. $C_{29}H_{38}O_3$

Testosterone phenylbutyrate

RN: **MP** (°C)**:**
MW: 434.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.681E-06	1.600E-03	25	L342	1 0 1 1 2	

4515. $C_{29}H_{40}N_2O_4$

Emetine
Emetan, 6′,7′,10,11-tetramethoxy-
NSC 33669

RN: 483-18-1 **MP** (°C)**:** 74
MW: 480.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	9.613E-01	15	K059	2 2 2 0 0	
2.078E-03	9.990E-01	c	D004	0 0 0 0 0	

4516. $C_{29}H_{42}O_6$

Cortisone caprylate

RN: **MP** (°C)**:**
MW: 486.65 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.110E-06	2.000E-03	25	M023	1 0 2 1 0	

4517. $C_{29}H_{44}FNO_{11}.H_2O$
N-Methylglucamine 9-α-fluorohyfrocortisome (monohydrate)
21-(9-α-Fluoro-11β, 17α-dihydroxy-4-pregnen-3,20-dione)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 120
MW: 619.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.358E-03	3.940E+00	25	L009	1 0 0 1 1	

4518. $C_{29}H_{44}O_{12}$
Oubain
γ-Strophanthin
Ouabain
Quabain
RN: 630-60-4 **MP** (°C)**:** 185
MW: 584.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.223E-02	1.300E+01	25	P312	0 0 0 0 0	
1.693E-02	9.901E+00	c	D004	0 0 0 0 0	
2.851E-01	1.667E+02	h	D004	0 0 0 0 0	

4519. $C_{29}H_{46}N_4O_7.0.4H_2O$
2′-(2-Octanoyl-2-heptanyl-acetyl)-6-methoxypurine arabinoside (0.4 hydrate)
RN: 145913-53-7 **MP** (°C)**:**
MW: 569.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.601E-02	37	C348	0 0 0 0 0	pH 7.00

4520. $C_{29}H_{46}O_3$
Nandrolone undecanoate
RN: **MP** (°C)**:**
MW: 442.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-06	6.020E-04	37	C026	0 0 0 0 0	

4521. $C_{29}H_{50}O_2$
Vitamin E
α-Tocopherol
RN: 59-02-9 **MP** (°C)**:**
MW: 430.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.833E-05	2.082E-02	33	D404	2 1 2 2 2	
4.852E-05	2.090E-02	33	D404	2 1 2 2 2	

4522. $C_{30}H_{28}N_4O_3$
Benzoyldiantipyrylmethane
BenzDAM
RN: 55774-17-9 **MP** (°C)**:**
MW: 492.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.03E-05	<1.00E-02	20	P054	0 0 0 0 0	

4523. $C_{30}H_{30}N_{20}O_{10}$
Cucurbit[5]uril
RN: 259886-49-2 **MP** (°C)**:**
MW: 830.70 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	3.406E-01	25	B424	1 0 1 2 2	

4524. $C_{30}H_{34}O_{13}$
Picrotoxin
Picrotoxine
RN: 124-87-8 **MP** (°C)**:**
MW: 602.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.964E-03	2.991E+00	20	D041	1 0 0 0 0	
6.776E-03	4.083E+00	rt	D021	0 0 1 1 1	

4525. $C_{30}H_{48}O_3$
β-Boswellic acid
RN: **MP** (°C)**:**
MW: 456.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	7.764E+00	ns	R422	0 0 0 0 0	

4526. $C_{30}H_{48}O_{12}$
Periplocin
Card-20(22)-enolide, 3-[(2,6-dideoxy-4-*O*-β-D-glucopyranosyl-3-*O*-methyl-β-D-ribo-hexopyranosyl)oxy]-5,14-dihydroxy-, (3β,5β)-
Periplocoside
RN: 13137-64-9 **MP** (°C)**:** 205
MW: 600.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.321E-02	7.937E+00	c	D004	0 0 0 0 0	

4527. $C_{31}H_{33}N_5O_2$
p-Dimethylaminophenyldiantipyrylmethane
p-DMAPhDAM
RN: 2088-76-8 **MP** (°C)**:**
MW: 507.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.576E-04	7.999E-02	20	P054	0 0 0 0 0	

4528. $C_{31}H_{38}N_2O_{11}$
Dihydronovobiocin
Benzamide, *N*-[7-[[3-*O*-(aminocarbonyl)-6-deoxy-5-C-methyl-4-*O*-methyl-β-L-lyxo-hexopyranosyl]oxy]-4-hydroxy-8-methyl-2-oxo-2H-1-benzopyran-3-yl]-4-hydroxy-3-(3-methylbutyl)-
RN: 29826-16-2 **MP** (°C)**:**
MW: 614.66 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.800E-01	28	A038	2 0 1 1 2	

4529. $C_{31}H_{42}FNO_{12}.H_2O$
Glucosamine triamcinolone acetonide (monohydrate)
21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-2-(2-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 250–255
MW: 657.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.717E-04	3.760E-01	25	L009	1 0 0 1 1	

4530. $C_{31}H_{44}FNO_{12}.H_2O$
Glucaminetriamcinolone acetonide (monohydrate)
21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 150
MW: 659.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.366E-03	3.540E+00	25	L009	1 0 0 1 1	

4531. $C_{31}H_{44}N_2O_7$
N-Acetyl-L-tyrosinamide prostaglandin E2
RN: **MP** (°C)**:**
MW: 556.71 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	9.464E-02	25	A066	1 0 1 1 1	

4532. $C_{31}H_{46}N_2O_7$
N-Acetyl-L-tyrosinamide prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 558.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	7.822E-02	25	A066	1 0 1 1 1	

4533. $C_{31}H_{48}O_{12}$
Strophanthin
k-Strophanthin
RN: 11005-63-3 **MP** (°C)**:** 179
MW: 612.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	2.273E+01	25	D004	0 0 0 0 0	

4534. $C_{32}H_{32}O_{14}$
Chartreusin
Lambdamycin
NSC 5159
Antibiotic X 465A
RN: 6377-18-0 **MP** (°C)**:** 246–249
MW: 640.60 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-05	1.500E-02	25	P067	0 0 0 0 0	

4535. $C_{32}H_{37}NO_5S$
Dextropropoxyphene napsylate
Darvocet N-50
Darvocet N-100
Darvon-N
RN: 17140-78-2 **MP** (°C)**:**
MW: 547.72 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-03	1.400E+00	22	N319	0 0 0 0 0	

4536. $C_{32}H_{40}BrN_5O_5$
Bromocriptine
2-Bromo-α-ergocryptine
Parlodel
Kripton
(5′α)-2-Bromo-12′-hydroxy-2′-(1-methylethyl)-5′-(2-methylpropyl)ergotaman-3′,6′,18-trione
RN: 25614-03-3 **MP** (°C)**:**
MW: 654.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-06	2.070E-03	ns	R427	0 0 0 0 0	

4537. $C_{32}H_{41}NO_2$
Terfenadine
Seldane
Teldane
RN: 50679-08-8 **MP** (°C)**:**
MW: 471.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-10	9.700E-08	25	A412	1 0 2 2 1	
		amb	L434	0 0 0 0 0	
2.138E-07	1.008E-04	ns	R427	0 0 0 0 0	

4538. $C_{32}H_{45}N_3O_4S$
Nelfinavir mesylate
Nelfinavir
NFV
Viracept
RN: 159989-65-8 **MP** (°C)**:**
MW: 567.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.925E-03	4.500E+00	ns	W424	0 0 0 0 0	

4539. $C_{32}H_{45}N_3O_4S$

Nelfinavir

(3*S*,4a*S*,8a*S*)-*N*-(1,1-Dimethylethyl)decahydro-2-[(2*R*,3*R*)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-(phenylthio)butyl]-3-isoquinolinecarboxamide

RN: 159989-64-7 **MP** (°C)**:**
MW: 567.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-02	7.000E+00	ns	A426	0 0 0 0 0	Intrinsic

4540. $C_{32}H_{46}FNO_{12}.H_2O$

N-Methylglucamine triamcinolone acetonide (monohydrate)

21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate

RN: **MP** (°C)**:** 152
MW: 673.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.744E-03	3.196E+00	25	L009	1 0 0 1 1	

4541. $C_{32}H_{49}NO_9$

Cevadine

Cevane-3,4,12,14,16,17,20-heptol, 4,9-epoxy-, 3-[(2Z)-2-methyl-2-butenoate], (3β,4α,16β)-

Veratrine

RN: 62-59-9 **MP** (°C)**:** 213.5
MW: 591.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	4.734E+00	15	K059	2 2 2 0 0	

4542. $C_{32}H_{54}O_4$

Didodecyl phthalate

1,2-Benzenedicarboxylic acid, didodecyl ester

RN: 2432-90-8 **MP** (°C)**:**
MW: 502.78 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-07	1.400E-04	24	H116	2 1 0 0 2	

4543. $C_{33}H_{25}N_3O_3$
Norbormide
5-(α-Hydroxy-α-2-pyridylbenzyl)-7-(α-2-pyridylbenzylidene)-5-norbornene-2,3-dicaboximide
Shoxin
RN: 991-42-4 **MP** (°C)**:** >160
MW: 511.59 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-04	6.000E-02	rt	M161	0 0 0 0 1	

4544. $C_{33}H_{34}O_3$
Norethindrone biphenyl-4-carboxylate
RN: **MP** (°C)**:**
MW: 478.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-09	3.715E-06	25	L078	1 0 1 2 2	

4545. $C_{33}H_{34}O_4$
Norethindrone 4-phenoxybenzoate
RN: **MP** (°C)**:**
MW: 494.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-07	7.079E-05	25	L078	1 0 1 2 2	

4546. $C_{33}H_{36}N_4O_6$
Bilirubin
21H-Biline-8,12-dipropanoic acid, 2,17-diethenyl-1,10,19,22,23,24-hexahydro-3,7,13,18-tetramethyl-1,19-dioxo-
RN: 635-65-4 **MP** (°C)**:**
MW: 584.68 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	4.093E-06	18	K104	1 0 0 0 2	intrinsic

4547. $C_{33}H_{40}N_2O_9$
Reserpine
3,4,5-Trimethoxybenzoyl methyl reserpate
Rauwilid
Rauwiloid
RN: 50-55-5 **MP** (°C)**:**
MW: 608.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	7.304E-02	30	L068	1 0 0 1 0	EFG
1.643E-05	1.000E-02	ns	K444	0 0 0 0 0	

4548. $C_{33}H_{41}N_5O_6S_2$
Kynostatin
KNI-272
4-Thiazolidinecarboxamide, *N*-(1,1-dimethylethyl)-3-[(2*S*,3*S*)-2-hydroxy-3-[[(2*R*)-2-[[(5-isoquinolinyloxy)acetyl]amino]-3-(methylthio)-1-oxopropyl]amino]-1-oxo-4-phenylbutyl]-, (4*R*)-
RN: 147318-81-8 **MP** (°C)**:**
MW: 667.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-06	4.200E-03	25	J308	0 0 0 0 0	

4549. $C_{33}H_{45}NO_9$
Delphinine
Indaconitine, *N*-deethyl-3-deoxy-*N*-methyl-
RN: 561-07-9 **MP** (°C)**:** 198–200
MW: 599.73 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.335E-05	2.000E-02	25	D004	0 0 0 0 0	

4550. $C_{33}H_{47}NO_{13}$
Natamycin
Pimafucin
RN: 7681-93-8 **MP** (°C)**:**
MW: 665.74 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-05	3.000E-02	20	B190	1 2 1 1 0	
6.159E-04	4.100E-01	21	M044	2 0 2 2 2	*sic*

4551. $C_{34}H_{30}N_2O_6S$

Pyrantel pamoate
Pirantel pamoate
Dog Wormer
Helmex
Lombriareu
Trilombrin

RN: 22204-24-6 **MP** (°C)**:** 266–267
MW: 594.69 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E-05	1.000E-02	ns	K444	0 0 0 0 0	

4552. $C_{34}H_{34}N_4O_4$

Protoprophyrin IX
Protoporphyrin IX

RN: 553-12-8 **MP** (°C)**:**
MW: 562.67 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	1.069E-01	25	C097	2 0 1 1 1	EFG

4553. $C_{34}H_{47}NO_{11}$

Aconitine
Acetylbenzoylaconine

RN: 302-27-2 **MP** (°C)**:** 204
MW: 645.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.691E-04	3.029E-01	25	D004	0 0 0 0 0	

4554. $C_{34}H_{50}O_7$

Carbenoxolone
Olean-12-en-29-oic acid, 3-(3-carboxy-1-oxopropoxy)-11-oxo-, (3β,20β)-

RN: 5697-56-3 **MP** (°C)**:**
MW: 570.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-05	6.621E-03	24	B363	0 0 0 0 0	
1.630E-05	9.304E-03	37	B363	0 0 0 0 0	

4555. $C_{34}H_{57}NO_7$
Glucosamine cholesterol
3-β-(5-Cholestenyl)-*N*-2-(2-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 155–158
MW: 591.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.530E-04	5.640E-01	25	L009	1 0 0 1 1	

4556. $C_{34}H_{58}O_4$
Ditridecyl phthalate
Staflex DTDP
Truflex DTDP
Hexaplas DTDP
Jayflex DTDP
Polycizer 962BPA
RN: 119-06-2 **MP** (°C)**:**
MW: 530.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.405E-07	3.400E-04	24	H116	2 1 0 0 2	

4557. $C_{34}H_{68}N_3O_8S_2$
Lincomycin hexadecylsulfamate
RN: **MP** (°C)**:**
MW: 711.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.738E-04	4.080E-01	21	M044	2 0 2 2 2	

4558. $C_{35}H_{44}N_2O_7$
p-(*p*-Acetamidobenzamido)phenyl prostaglandin E2
RN: **MP** (°C)**:**
MW: 604.75 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-08	5.927E-05	25	A066	1 0 1 1 1	

4559. $C_{35}H_{46}N_2O_7$
p-(*p*-Acetamidobenzamido)phenyl prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 606.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-07	1.699E-04	25	A066	1 0 1 1 1	

4560. $C_{35}H_{47}NO_9$
Rhizoxin
RN: 90996-54-6 **MP** (°C)**:**
MW: 625.77 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-05	1.200E-02	25	P336	0 0 0 0 0	

4561. $C_{35}H_{61}NO_7$
N-Methylglucamine cholesterol
3-β-(5-Cholestenyl)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate
RN: **MP** (°C)**:** 131–133
MW: 607.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-04	1.120E-01	25	L009	1 0 0 1 1	

4562. $C_{36}H_{47}N_2O_7$
N-Benzoyl-L-tyrosinamide prostaglandin E2
RN: **MP** (°C)**:**
MW: 619.79 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-07	2.913E-04	25	A066	1 0 1 1 1	

4563. $C_{36}H_{47}N_5O_4$
Indinavir sulfate
Crixivan
IDV
Indinavir
Indinavir sulfate
MK-639
RN: 157810-81-6 **MP** (°C)**:**
MW: 613.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.63E-01	>1.00E+02	ns	W424	0 0 0 0 0	

4564. $C_{36}H_{47}N_5O_4$
Indinavir
2,3,5-Trideoxy-*N*-[(1*S*,2*R*)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]-5-[(2*S*)-2-[[(1,1-dimethylethyl) amino]carbonyl]-4-(3-pyridinylmethyl)-1-piperazinyl]-2-(phenylmethyl)-D-erythro-pentonamide
N-(2-hydroxy-1(*S*)-indanyl)-2-(phenylmethyl)-4(*S*)-hydroxy-5-[1-[4-(3-pyridylmethyl)-2(*S*)-(*N*-*tert*-butylcarbamoyl)piperazinyl]]pentanamide
RN: 150378-17-9 **MP** (°C)**:**
MW: 613.81 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	7.000E-02	ns	A426	0 0 0 0 0	Intrinsic

4565. $C_{36}H_{49}N_2O_7$
N-Benzoyl-L-tyrosinamide prostaglandin F2 α
RN: **MP** (°C)**:**
MW: 621.80 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	1.119E-03	25	A066	1 0 1 1 1	

4566. $C_{36}H_{56}O_{14}$
Digitalin
Card-20(22)-enolide, 3-[(6-deoxy-4-*O*-β-D-glucopyranosyl-3-*O*-methyl-β-D-galactopyranosyl) oxy]-14,16-dihydroxy-, (3β,5β,16β)-
Digitalinum verum
RN: 752-61-4 **MP** (°C)**:** 229
MW: 712.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.401E-03	9.990E-01	25	D004	0 0 0 0 0	

4567. $C_{36}H_{57}N_7O_{10}S$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(2-sulfoethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-, [1*S*-[1*R**,2*R**,4(*R**)]]-

RN: 100902-06-5 **MP** (°C)**:**
MW: 779.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.10E-02	>8.58E+00	ns	B425	0 0 0 1 0	

4568. $C_{36}H_{58}N_8O_7$

L-Leucinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3*S*,4*S*)-4-amino-3-hydroxy-6-methylheptanoyl-*N*-(2-aminoethyl)-

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[(2-aminoethyl)amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 105192-87-8 **MP** (°C)**:**
MW: 714.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	3.503E+00	ns	B425	0 0 0 1 0	pH 7.4

4569. $C_{36}H_{60}O_2$

Vitamin A palmitate
Retinol, hexadecanoate
Retinyl palmitate

RN: 79-81-2 **MP** (°C)**:**
MW: 524.88 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.624E-04	25	P343	0 0 0 0 0	
1.905E-05	1.000E-02	ns	K444	0 0 0 0 0	

4570. $C_{36}H_{60}O_{30}$

α-Cyclodextrin
β-Hexaamylose
(C6H10O5)6
α-Dextrin

RN: 10016-20-3 **MP** (°C)**:**
MW: 972.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.345E-02	9.091E+01	20	F186	1 2 1 1 1	
2.409E-02	2.344E+01	20	P048	1 0 1 1 1	*sic*
1.118E-01	1.088E+02	23.7	J305	0 0 0 0 0	
1.204E-01	1.171E+02	23.7	J305	0 0 0 0 0	
1.460E-01	1.420E+02	25	B396	0 0 0 0 0	

(*continued*)

4570. $C_{36}H_{60}O_{30}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-01	1.450E+02	25	L432	0 0 0 0 0	
1.800E-01	1.751E+02	25	O321	0 0 0 0 0	
1.331E-01	1.295E+02	25	S462	0 0 0 0 0	
1.211E-01	1.178E+02	25.0	J305	0 0 0 0 0	
1.318E-01	1.282E+02	25.0	J305	0 0 0 0 0	
1.678E-01	1.632E+02	30.0	J305	0 0 0 0 0	
1.501E-01	1.460E+02	30.0	J305	0 0 0 0 0	
1.696E-01	1.650E+02	33.0	J305	0 0 0 0 0	
1.912E-01	1.860E+02	33.0	J305	0 0 0 0 0	
2.161E-01	2.102E+02	35.0	J305	0 0 0 0 0	
1.885E-01	1.834E+02	35.0	J305	0 0 0 0 0	
2.331E-01	2.268E+02	38.0	J305	0 0 0 0 0	
2.023E-01	1.968E+02	38.0	J305	0 0 0 0 0	
2.100E-01	2.043E+02	40	O321	0 0 0 0 0	
2.171E-01	2.112E+02	40.0	J305	0 0 0 0 0	
2.532E-01	2.463E+02	40.0	J305	0 0 0 0 0	
2.229E-01	2.169E+02	42.0	J305	0 0 0 0 0	
2.616E-01	2.545E+02	42.0	J305	0 0 0 0 0	
2.677E-01	2.604E+02	43.0	J305	0 0 0 0 0	
2.283E-01	2.221E+02	43.0	J305	0 0 0 0 0	
2.492E-01	2.424E+02	45.0	J305	0 0 0 0 0	
2.982E-01	2.901E+02	45.0	J305	0 0 0 0 0	
3.397E-01	3.305E+02	48.0	J305	0 0 0 0 0	
2.773E-01	2.698E+02	48.0	J305	0 0 0 0 0	
4.700E-01	4.572E+02	55	O321	0 0 0 0 0	
1.302E-01	1.266E+02	ns	M335	0 0 2 0 1	
1.490E-01	1.450E+02	rt	F041	0 2 2 0 2	

4571. $C_{36}H_{72}N_3O_8S_2$

Lincomycin octadecylsulfamate

RN: **MP** (°C)**:**

MW: 739.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.897E-04	2.880E-01	21	M044	2 0 2 2 2	

4572. $C_{36}H_{74}$

n-Hexatriacontane

Hexatriacontane

RN: 630-06-8 **MP** (°C)**:** 75.0

MW: 506.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-09	1.700E-06	25	B069	1 0 1 1 1	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 2	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 0	

4573. $C_{37}H_{48}N_6O_5S_2$
Ritonavir
ABT-538
Norvir
Ritonavir
RN: 155213-67-5 **MP** (°C)**:**
MW: 720.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.935E-06	5.000E-03	ns	A426	0 0 0 0 0	intrinsic
1.387E-05	1.000E-02	ns	K444	0 0 0 0 0	
~1.39E+00	~9.99E+02	ns	W424	0 0 0 0 0	

4574. $C_{37}H_{67}NO_{13}.2H_2O$
Erythromycin (dihydrate)
RN: 114-07-8 **MP** (°C)**:**
MW: 769.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.857E-04	5.280E-01	30	F310	1 0 2 2 2	
4.922E-04	3.790E-01	40	F310	1 0 2 2 2	
4.377E-04	3.370E-01	50	F310	1 0 2 2 2	
4.143E-04	3.190E-01	60	F310	1 0 2 2 2	
4.598E-04	3.540E-01	70	F310	1 0 2 2 2	
5.688E-04	4.380E-01	80	F310	1 0 2 2 2	

4575. $C_{38}H_{50}N_6O_5$
Squinavir
Butanediamide, *N*1-[(1*S*,2*R*)-3-[(3*S*,4a*S*,8a*S*)-3-[[(1,1-dimethylethyl)amino]carbonyl]octahydro-2-(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-
Saquinavir mesylate
Fortovase
Invirase
(*S*)-*N*-[(a*S*)-a-[(1*R*)-2-[(3*S*,4a*S*,8a*S*)-3-(*tert*-Butylcarbamoyl)octahydro-2(1H)-isoquinolyl]-1-hydroxyethyl]phenethyl]-2-quinaldamidosuccinamide
RN: 127779-20-8 **MP** (°C)**:**
MW: 670.86 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.336E-05	3.580E-02	25	B431	1 0 1 1 0	
8.198E-05	5.500E-02	25	C437	0 0 0 0 0	Average
3.309E-03	2.220E+00	ns	W424	0 0 0 0 0	

4576. $C_{38}H_{60}N_8O_9$

Butanoic acid, *N*4-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-2,4-diamino-

RN: 115511-05-2 **MP** (°C)**:**
MW: 772.95 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	1.778E+00	ns	B425	0 0 0 1 0	pH 7.4

4577. $C_{38}H_{69}NO_{13}$

Clarithromycin
Biaxin
A-56268
TE-031

RN: 81103-11-9 **MP** (°C)**:** 218.5
MW: 747.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-04	9.948E-02	20	N334	0 0 0 0 0	EFG
1.089E-04	8.145E-02	37	N334	0 0 0 0 0	EFG
4.893E-05	3.660E-02	50	N334	0 0 0 0 0	EFG

4578. $C_{40}H_{51}NO_{14}$

Streptovaricin C
Streptovaricin

RN: 1404-74-6 **MP** (°C)**:** 189
MW: 769.85 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.604E-03	1.235E+00	21	M044	2 0 2 2 2	

4579. $C_{40}H_{58}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(2-pyridinylmethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-49-4 **MP** (°C)**:**
MW: 762.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	1.373E-01	ns	B425	0 0 0 1 0	pH 7.4

4580. $C_{40}H_{58}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[(4-pyridinylmethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-50-7 **MP** (°C)**:**
MW: 762.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	2.594E-01	ns	B425	0 0 0 1 0	pH 7.4

4581. $C_{40}H_{58}N_8O_8$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[[(1-oxido-4-pyridinyl)methyl]amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100902-03-2 **MP** (°C)**:**
MW: 778.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	3.272E+00	ns	B425	0 0 0 1 0	pH 7.4

4582. $C_{41}H_{59}N_7O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[(phenylmethyl)amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 109585-11-7 **MP** (°C)**:**
MW: 761.97 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<7.62E-03	ns	B425	0 0 0 1 0	pH 7.4

4583. $C_{41}H_{61}N_9O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[2-amino-2-(2-pyridinyl)ethyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-99-3 **MP** (°C)**:**
MW: 792.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	3.168E-01	ns	B425	0 0 0 1 0	pH 7.4

4584. $C_{41}H_{64}O_{13}$

Digitoxin
(3β,5β)-3-[(0-2,6-Dideoxy-β-D-ribo-hexopyranosyl-(1->4)-*O*-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1->4)-2,6-dideoxy-β-D-ribo-hexopyranosyl)oxy]-14-hydroxycard-20(22)-enolide
Crystodigin
Digifortis
RN: 71-63-6 **MP** (°C)**:** 256
MW: 764.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.307E-05	1.000E-02	20	J010	1 0 0 0 0	
5.098E-06	3.900E-03	25	M301	1 1 2 2 1	anhydrate
2.000E-05	1.530E-02	30	O321	0 0 0 0 0	
2.222E-05	1.700E-02	30	O321	0 0 0 0 0	
1.447E-05	1.107E-02	37	C303	2 2 2 2 2	average of 3
3.255E-06	2.490E-03	37	M301	1 1 2 2 1	anhydrate
1.300E-05	9.944E-03	ns	M070	0 0 0 0 1	
9.151E-06	7.000E-03	ns	N302	0 2 1 2 0	

4585. $C_{41}H_{64}O_{14}$

Digoxin
3β-((*O*-2,6-Dideoxy-β-D-ribo-hexopyranosyl-(1->4)-*O*-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1->4)-2,6-dideoxy-β-D-ribo-hexopyranosyl)oxy)-12β,14-dihydroxy-5β-card-20(22)-enolide
Lanoxicaps
Lanoxin
RN: 20830-75-5 **MP** (°C)**:** 260
MW: 780.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	9.789E-02	25	F010	2 1 2 2 2	Swiss micron
6.786E-05	5.300E-02	25	F010	2 1 2 2 2	
7.375E-05	5.760E-02	25	F010	2 1 2 2 2	Swiss standard
8.297E-05	6.480E-02	25	F010	2 1 2 2 2	
1.000E-04	7.810E-02	25	H066	1 0 0 0 0	EFG
3.585E-05	2.800E-02	25	M301	1 1 2 2 1	
3.675E-05	2.870E-02	25	N301	2 0 2 2 2	
3.841E-05	3.000E-02	27	E052	2 0 2 2 0	EFG
3.585E-05	2.800E-02	30	O321	0 0 0 0 0	
4.000E-05	3.124E-02	30	O321	0 0 0 0 0	
6.312E-05	4.930E-02	37	C303	2 2 2 2 2	average of 6
3.457E-05	2.700E-02	37	M301	1 1 2 2 1	
3.483E-05	2.720E-02	37	N301	2 0 2 2 2	
4.443E-05	3.470E-02	37	R009	1 0 0 0 2	
2.817E-05	2.200E-02	100	D027	1 2 0 0 1	
1.268E-03	9.900E-01	amb	L434	0 0 0 0 0	
7.363E-06	5.750E-03	ns	F037	0 0 2 0 2	mp 225.5 C
8.963E-06	7.000E-03	ns	F037	0 0 2 0 2	mp 225.5 C
5.570E-06	4.350E-03	ns	F037	0 0 2 0 2	mp 228.5 C

(*continued*)

4585. $C_{41}H_{64}O_{14}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.915E-06	5.400E-03	ns	F037	0 0 2 0 2	mp 235.5 C
1.280E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.097E-05	3.200E-02	ns	N302	0 2 1 2 1	
5.900E-05	4.608E-02	rt	J034	0 0 0 0 0	

4586. $C_{41}H_{64}O_{14}$

Gitoxin
Anhydrogitalin
Pseudodigitoxin
Bigitalin

RN: 4562-36-1 **MP** (°C)**:**
MW: 780.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	2.343E-03	ns	M070	0 0 0 0 0	

4587. $C_{41}H_{67}NO_{15}$

Troleandomycin
Triacetyloleandomycin

RN: 2751-09-9 **MP** (°C)**:**
MW: 813.99 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.071E-04	2.500E-01	28	A038	2 0 1 1 1	

4588. $C_{41}H_{68}N_8O_9$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[3-[bis(2-hydroxyethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 87691-52-9 **MP** (°C)**:**
MW: 817.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	3.513E+00	ns	B425	0 0 0 1 0	

4589. $C_{42}H_{59}N_7O_9$

Glycine, *N*-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-D-2-phenyl-

RN: 115511-06-3 **MP** (°C)**:**
MW: 805.98 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-04	5.964E-01	ns	B425	0 0 0 1 0	

4590. $C_{42}H_{62}N_8O_7$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-98-2 **MP** (°C)**:**
MW: 791.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	1.107E+00	ns	B425	0 0 0 1 0	pH 7.4

4591. $C_{42}H_{70}O_{35}$

β-Cyclodextrin
β-Cyclodextrin hydrate
Cycloheptaamylose hydrate
Cyclodextrin hydrate

RN: 7585-39-9 **MP** (°C)**:** 298–300
MW: 1135.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-02	1.185E+01	15	W317	2 2 1 0 2	
1.216E-02	1.381E+01	20	F186	1 2 1 1 1	
1.282E-02	1.455E+01	20	W317	2 2 1 0 2	
1.410E-02	1.600E+01	21	C407	1 0 1 2 1	
1.540E-02	1.748E+01	23.7	J305	0 0 0 0 0	
1.630E-02	1.850E+01	25	B396	0 0 0 0 0	
1.586E-02	1.800E+01	25	C407	1 0 1 2 1	
1.558E-02	1.768E+01	25	H319	0 0 0 0 0	
1.600E-02	1.816E+01	25	O304	1 2 2 2 2	
1.600E-02	1.816E+01	25	O321	0 0 0 0 0	
1.621E-02	1.840E+01	25	S462	0 0 0 0 0	
1.674E-02	1.900E+01	25	T425	0 0 0 0 0	
1.551E-02	1.760E+01	25	W317	2 2 1 0 2	
1.630E-02	1.850E+01	25.0	J305	0 0 0 0 0	
2.026E-02	2.300E+01	30	C407	1 0 1 2 1	
1.895E-02	2.151E+01	30	W317	2 2 1 0 2	
2.203E-02	2.500E+01	35	C407	1 0 1 2 1	
2.440E-02	2.769E+01	35.0	J305	0 0 0 0 0	
3.100E-02	3.519E+01	40	O321	0 0 0 0 0	
2.980E-02	3.382E+01	40.0	J305	0 0 0 0 0	

(*continued*)

4591. $C_{42}H_{70}O_{35}$ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.850E-02	4.370E+01	45.0	J305	0 0 0 0 0	
4.430E-02	5.028E+01	48.0	J305	0 0 0 0 0	
4.400E-02	4.994E+01	55	O321	0 0 0 0 0	
1.558E-02	1.768E+01	ns	M335	0 0 2 0 1	

4592. $C_{42}H_{70}O_{35}$

6-*O*-α-D-Glucosyl-α-cyclodextrin

RN: **MP** (°C)**:**

MW: 1135.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-01	9.080E+02	25	O321	0 0 0 0 0	
1.030E+00	1.169E+03	40	O321	0 0 0 0 0	
1.190E+00	1.351E+03	55	O321	0 0 0 0 0	

4593. $C_{43}H_{55}NO_{13}$

Docetaxel

Taxotere

N-Debenzoyl-*N*-*tert*-butoxycarbonyl-10-deacetyl taxol

RN: 114977-28-5 **MP** (°C)**:**

MW: 793.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.557E-06	6.000E-03	22.5	C438	0 0 0 0 0	

4594. $C_{43}H_{58}N_4O_{12}$

Rifampin

Rifampicin

RN: 13292-46-1 **MP** (°C)**:**

MW: 822.96 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-01	1.070E+02	25	B073	2 1 2 2 2	pH 2.12,*sic*
4.374E-03	3.600E+00	25	B073	2 1 2 2 1	pH 2.5
1.701E-03	1.400E+00	25	B073	2 1 2 2 1	pH 5.33
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.99
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.03
1.580E-03	1.300E+00	25	G096	1 0 0 0 0	pH 4.3
1.215E-04	1.000E-01	ns	K444	0 0 0 0 0	
3.393E-03	2.792E+00	rt	F182	0 0 0 0 1	pH 7.5

4595. $C_{43}H_{61}N_7O_{10}$

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[[3-(carboxymethoxy) phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-, [1*S*-[1*R**,2*R**,4(*R**)]]-

RN: 100902-05-4 **MP** (°C)**:**
MW: 836.01 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	2.257E-01	ns	B425	0 0 0 1 0	

4596. $C_{43}H_{62}N_8O_7$

L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-*N*-[3-methyl-1-[[(4-pyridinylmethyl)amino]carbonyl]butyl]-

RN: 105192-86-7 **MP** (°C)**:**
MW: 803.02 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.03E-03	ns	B425	0 0 0 1 0	pH 7.4

4597. $C_{43}H_{62}N_8O_8$

L-Phenylalaninamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3*S*,4*S*)-4-amino-3-hydroxy-6-methylheptanoyl-L-leucyl-

L-Phenylalaninamide, *N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl] amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl-,

RN: **MP** (°C)**:**
MW: 819.02 **BP** (°C)**:** 1171.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-05	<1.64E-02	ns	B425	0 0 0 1 0	pH 7.4

4598. $C_{43}H_{75}NO_{16}$

Erythromycin ethyl succinate

RN: 1264-62-6 **MP** (°C)**:**
MW: 862.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	1.950E-01	21	M044	2 0 2 2 2	

4599. $C_{44}H_{56}O_4$

p-tert-Butylcalix[4]arenetetrol
Tetra-*p-tert*-butyltetracalix[4]arene
p-tert-Butylcalix[4]arene
p-tert-Butylcalix[4]arene-25,26,27,28-tetrol
Formaldehyde-*p-tert*-butylphenyl cyclic tetramer
5,11,17,23-Tetra-*p-tert*-butyl-25,26,27,28-tetrahydroxycalix(4)arene

RN: 60705-62-6 **MP** (°C)**:** 342–346
MW: 648.93 **BP** (°C)**:** 683.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<6.49E-03	25	B424	1 0 1 2 2	

4600. $C_{44}H_{64}N_8O_9$

D-Phenylalanine, 3-(aminomethyl)-*N*-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-

RN: 115511-03-0 **MP** (°C)**:**
MW: 849.05 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	3.311E-01	ns	B425	0 0 0 1 0	pH 7.4

4601. $C_{44}H_{69}NO_{10}$

Tacrolimus
FK506

RN: 104987-11-3 **MP** (°C)**:**
MW: 772.04 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-06	1.220E-03	25	A410	1 0 2 2 1	

4602. $C_{44}H_{74}O_{34}$

n-Ethyl-paba-β-cyclodextrin

RN: **MP** (°C)**:**
MW: 1147.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-03	5.850E+00	ns	F327	0 0 1 2 2	

4603. $C_{44}H_{74}O_{35}$
Hydroxyethyl-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1163.06 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-01	3.750E+02	ns	M335	0 0 2 0 1	

4604. $C_{45}H_{63}Cl_2NO_6$
Cosalane
RN: 154212-56-3 **MP** (°C)**:** 262 C
MW: 784.91 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.784E-09	1.400E-06	ns	V417	0 0 0 0 0	

4605. $C_{45}H_{66}N_8O_7$
L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[4-(phenylmethyl)-1-piperazinyl]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-
RN: 105192-85-6 **MP** (°C)**:**
MW: 831.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.31E-03	ns	B425	0 0 0 1 0	pH 7.4

4606. $C_{45}H_{66}N_8O_7$
L-threo-Pentonamide, *N*-[1-[[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]-5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-
RN: 100902-07-6 **MP** (°C)**:**
MW: 831.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	1.662E-02	ns	B425	0 0 0 1 0	pH 7.4

4607. $C_{45}H_{73}NO_{15}$
Solanine
β-D-Galactopyranoside, (3β)-solanid-5-en-3-yl *O*-6-deoxy-α-L-mannopyranosyl-(1®2)-*O*-[β-D-glucopyranosyl-(1-3)]-
Solanidane, β-D-galactopyranoside deriv
RN: 20562-02-1 **MP** (°C)**:**
MW: 868.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.604E-02	15	K059	2 2 2 0 0	

4608. $C_{45}H_{76}O_{35}$
n-Propyl-paba-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1177.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	2.472E+00	ns	F327	0 0 1 2 2	

4609. $C_{46}H_{62}N_4O_{11}$
Rifabutin
1′,4-Didehydro-1-deoxy-1,4-dihydro-5′-(2-methylpropyl)-1-oxo
Ansamycin
Antibiotic LM 427
LM 427
Mycobutin
RN: 72559-06-9 **MP** (°C)**:**
MW: 847.03 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E-04	1.900E-01	ns	S469	0 0 0 0 0	

4610. $C_{46}H_{65}N_7O_{10}$
Acetic acid, [3-[[[2-[[5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-L-threo-pentonoyl]amino]-4-methyl-1-oxopentyl]amino]methyl]phenoxy]-
RN: 100902-09-8 **MP** (°C)**:**
MW: 876.07 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.628E-02	ns	B425	0 0 0 1 0	

4611. $C_{46}H_{77}NO_{17}$
Tylosin
Vubityl 200
Vetil(R)
RN: 1401-69-0 **MP** (°C)**:** 128
MW: 916.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.195E-03	7.508E+00	21	M044	2 0 2 2 2	

4612. $C_{46}H_{78}O_{35}$
n-Butyl-paba-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1191.11 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	8.338E-01	ns	F327	0 0 1 2 2	

4613. $C_{47}H_{51}NO_{14}$
Paclitaxel
5-β,20-Epoxy-1,2-α,4,7-β,10-β,13-α-hexahydroxy-tax-11-en-9-one 4,10-diacetate 2-benzoate 13-ester with (2*R*,3*S*)-*N*-benzoyl-3-phenyl-isoserine
TAX
Taxal
Taxol
Taxol A
RN: 33069-62-4 **MP** (°C)**:** 213–216
MW: 853.93 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-07	3.000E-04	37	L435	0 0 0 0 0	
1.569E-06	1.340E-03	37	V412	0 0 0 0 0	

4614. $C_{47}H_{73}NO_{17}$
Amphotericin B
RN: 1397-89-3 **MP** (°C)**:**
MW: 924.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.116E-04	7.500E-01	28	A038	2 0 1 1 1	
3.246E-06	3.000E-03	ns	K067	0 0 2 1 0	intrinsic

4615. $C_{47}H_{75}NO_{17}$

Nystatin
Mycostatin
Biofanal
Nystex
Fungicidin

RN: 1400-61-9 **MP** (°C)**:**
MW: 926.12 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	3.600E-01	24	M166	2 0 0 0 1	
4.319E-03	4.000E+00	ns	K444	0 0 0 0 0	

4616. $C_{48}H_{72}O_{14}$

Ivermectin
Heartgard-30
Ivomec

RN: 70288-86-7 **MP** (°C)**:**
MW: 873.10 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-06	4.000E-03	ns	K444	0 0 0 0 0	

4617. $C_{48}H_{80}O_{40}$

6-*O*-α-D-Maltosyl-α-cyclodextrin
6-*O*-α-Maltosyl-α-cyclodextrin

RN: **MP** (°C)**:**
MW: 1297.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-01	9.988E+02	25	O321	0 0 0 0 0	
2.400E-01	3.113E+02	25	O321	0 0 0 0 0	
7.700E-01	9.988E+02	40	O321	0 0 0 0 0	
3.500E-01	4.540E+02	40	O321	0 0 0 0 0	
1.330E+00	1.725E+03	55	O321	0 0 0 0 0	
5.400E-01	7.005E+02	55	O321	0 0 0 0 0	

4618. $C_{48}H_{80}O_{40}$

γ-Cyclodextrin
Cyclooctaamylose
Ringdex C
Cyclomaltooctaose
Dexy Pearl γ-100

RN: 17465-86-0 **MP** (°C)**:**
MW: 1297.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.338E-01	1.736E+02	20	F186	1 2 1 1 1	
1.789E-01	2.320E+02	25	B396	0 0 0 0 0	
2.000E-01	2.594E+02	25	O321	0 0 0 0 0	
1.921E-01	2.492E+02	25	S462	0 0 0 0 0	
1.680E-01	2.179E+02	25.0	J305	0 0 0 0 0	
2.040E-01	2.646E+02	30.0	J305	0 0 0 0 0	
2.430E-01	3.152E+02	35.0	J305	0 0 0 0 0	
4.300E-01	5.578E+02	40	O321	0 0 0 0 0	
2.680E-01	3.476E+02	40.0	J305	0 0 0 0 0	
3.110E-01	4.034E+02	42.0	J305	0 0 0 0 0	
6.400E-01	8.302E+02	55	O321	0 0 0 0 0	
1.452E-01	1.883E+02	ns	M335	0 0 2 0 1	

4619. $C_{49}H_{87}NS$

Erythromycin lactobionate

RN: 3847-29-8 **MP** (°C)**:** 145
MW: 722.31 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.77E-02	>2.00E+01	21	M044	2 0 2 2 0	

4620. $C_{50}H_{82}N_{10}O_{31}S_{10}$

Decane(*S*-(carboxymethyl)-L-cysteine))

RN: **MP** (°C)**:**
MW: 1639.90 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E-05	9.544E-02	15	N331	0 0 0 0 0	
5.730E-04	9.397E-01	25	N331	0 0 0 0 0	

4621. $C_{51}H_{55}NO_{18}$
7-Malyl paclitaxel
RN: 265659-44-7 **MP** (°C)**:** 166–168
MW: 970.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.093E-04	3.000E-01	ns	D401	0 2 2 2 0	

4622. $C_{51}H_{55}NO_{18}$
2′-Malyl paclitaxel
RN: 265659-38-9 **MP** (°C)**:** 148–151
MW: 970.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-04	2.000E-01	ns	D401	0 2 2 2 0	

4623. $C_{51}H_{70}N_{12}O_{11}$
His-pro-D-phe-his-leu-leu-thr-tyr
RN: **MP** (°C)**:**
MW: 1027.20 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-05	8.320E-02	20	B141	1 2 0 0 1	pH 7.5

4624. $C_{51}H_{74}O_{19}$
Penta-acetyl-gitoxin
RN: 7242-04-8 **MP** (°C)**:**
MW: 991.15 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	1.189E-02	ns	M070	0 0 0 0 1	

4625. $C_{52}H_{72}N_{12}O_{10}$
His-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1025.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-04	1.651E-01	ns	B141	0 2 0 0 2	pH 7.5

4626. $C_{52}H_{72}N_{12}O_{10}$
His-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1025.23 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	1.405E-01	ns	B141	0 2 0 0 2	pH 7.5

4627. $C_{52}H_{88}O_{39}$
n-Butyl-paba-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1337.26 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	9.361E-01	ns	F327	0 0 1 2 2	

4628. $C_{52}H_{97}NO_{18}S$
Erythromycin estolate
RN: 3521-62-8 **MP** (°C)**:** 135
MW: 1056.41 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.515E-04	1.600E-01	21	M044	2 0 2 2 2	

4629. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Glucosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-01	1.430E+03	25	O321	0 0 0 0 0	
1.010E+00	1.474E+03	40	O321	0 0 0 0 0	
1.180E+00	1.722E+03	55	O321	0 0 0 0 0	

4630. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Maltosyl-β-cyclodextrin
6-*O*-α-Maltosyl-β-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.518E+03	25	O321	0 0 0 0 0	
1.040E+00	1.518E+03	40	O321	0 0 0 0 0	
1.220E+00	1.780E+03	55	O321	0 0 0 0 0	

4631. $C_{54}H_{90}O_{45}$
6-*O*-α-D-Maltotriosyl-α-cyclodextrin
6-*O*-α-Maltotriosyl-α-cyclodextrin
RN: **MP** (°C)**:**
MW: 1459.29 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E+00	1.561E+03	25	O321	0 0 0 0 0	
1.220E+00	1.780E+03	40	O321	0 0 0 0 0	
1.370E+00	1.999E+03	55	O321	0 0 0 0 0	

4632. $C_{55}H_{59}NO_{22}$
2′,7-*bis*-(Malyl) paclitaxel
RN: 265659-41-4 **MP** (°C)**:** 166–168
MW: 1086.08 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.604E-04	5.000E-01	ns	D401	0 2 2 2 0	

4633. $C_{55}H_{70}N_{12}O_{10}$
His-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1059.25 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-04	1.864E-01	ns	B141	0 2 0 0 2	pH 7.5

4634. $C_{55}H_{79}N_{13}O_{11}$
His-pro-D-phe-his-leu-leu-val-tyr-serinol
RN: **MP** (°C)**:**
MW: 1098.32 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.295E-01	20	B141	1 2 0 0 2	pH 7.5

4635. $C_{55}H_{90}N_{11}O_{34}S_{11}$
Undecane(*S*-(carboxymethyl)-L-cysteine))
RN: **MP** (°C)**:**
MW: 1802.09 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-06	1.658E-02	15	N331	0 0 0 0 0	
1.340E-04	2.415E-01	25	N331	0 0 0 0 0	
2.900E-04	5.226E-01	35	N331	0 0 0 0 0	

4636. $C_{56}H_{98}O_{35}$
β-Cyclodextrin, tetradeca-*O*-methyl-
Heptakis(2,6-di-*O*-methyl)-β-cyclodextrin
RN: 188367-19-3 **MP** (°C)**:**
MW: 1331.38 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-01	3.631E+02	25	H319	0 0 0 0 0	

4637. $C_{57}H_{79}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1122.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.240E-04	3.636E-01	ns	B141	0 2 0 0 2	pH 7.5

4638. $C_{57}H_{79}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1122.35 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	4.602E-02	ns	B141	0 2 0 0 1	pH 7.5

4639. $C_{60}H_{77}N_{13}O_{11}$
Pro-his-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1156.36 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-04	3.966E-01	ns	B141	0 2 0 0 2	pH 7.5

4640. $C_{60}H_{92}N_{12}O_{10}$
Gramicidin S
Gramicidin
Cyclo(L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl-L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl)
Gramicidin S-A
RN: 113-73-5 **MP** (°C)**:**
MW: 1141.48 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-04	1.400E-01	28	A038	2 0 1 1 2	

4641. $C_{60}H_{98}N_{12}O_{37}S_{12}$
Dodecane(*S*-(carboxymethyl)-L-cystein))
RN: **MP** (°C)**:**
MW: 1964.28 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	4.518E-03	15	N331	0 0 0 0 0	
2.400E-05	4.714E-02	25	N331	0 0 0 0 0	
5.880E-05	1.155E-01	35	N331	0 0 0 0 0	

4642. $C_{60}H_{100}O_{50}$
6-*O*-α-D-Maltotriosyl-β-cyclodextrin
6-*O*-α-Maltotriosyl-β-cyclodextrin
6-*O*-α-D-Maltosyl-γ-cyclodextrin
6-*O*-α-Maltosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1621.44 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-01	1.524E+03	25	O321	0 0 0 0 0	
9.400E-01	1.524E+03	40	O321	0 0 0 0 0	
1.140E+00	1.848E+03	55	O321	0 0 0 0 0	
1.100E+00	1.784E+03	55	O321	0 0 0 0 0	

4643. $C_{62}H_{86}N_{12}O_{16}$
Actinomycin D
Actactinomycin A IV
Actinomycin AIV
Actinomycin I1
RN: 50-76-0 **MP** (°C)**:**
MW: 1255.45 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.983E-04	5.000E-01	37	G025	1 0 0 0 1	
7.965E-04	1.000E+00	rt	G025	0 0 0 0 1	

4644. $C_{62}H_{111}N_{11}O_{12}$
Cyclosporin A
1,4,7,10,13,16,19,22,25,28,31-Undecaazacyclotritriacontane, cyclic peptide deriv.
Sandimmun neoral
Sandimmun
Sang-35
SDZ-OXL 400
RN: 59865-13-3 **MP** (°C)**:** 148–151
MW: 1202.64 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.326E-05	4.000E-02	25	B376	0 0 0 0 0	
8.315E-06	1.000E-02	amb	L434	0 0 0 0 0	

4645. $C_{63}H_{85}N_{21}O_{19}$
Candicidin
Candeptin
Vanobid
RN: 1403-17-4 **MP** (°C)**:**
MW: 1440.51 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.349E-03	1.347E+01	21	M044	2 0 2 2 2	

4646. $C_{63}H_{88}N_{14}O_{14}PCo$
Vitamin B12
Cyanoject
Hydrobexan
Alphamine
Crystamine
Cyomin
RN: 68-19-9 **MP** (°C)**:**
MW: 1355.40 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.149E-03	1.240E+01	20	F300	1 0 0 0 2	

4647. $C_{64}H_{112}O_{40}$
Dimethyl-β-cyclodextrin
β-Cyclodextrin, 2A,2B,2C,2D,2E,2F,2G,6A,6B,6C,6D,6E,6F,6G-Tetradeca-*O*-methyl-
Heptakis(2,6-di-*O*-methyl)-β-cyclodextrin
Tetradeca-*O*-methyl-β-cyclodextrin
Tetradecakis-2,6-*O*-methylcycloheptaamylose
RN: 51166-71-3 **MP** (°C)**:** 298–300
MW: 1521.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	2.126E+02	c	D316	0 0 0 0 0	

4648. $C_{65}H_{106}N_{13}O_{40}S_{13}$
Tridecane(*S*-(carboxymethyl)-L-cyateine))
RN: **MP** (°C)**:**
MW: 2126.46 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.318E-02	25	N331	0 0 0 0 0	
1.600E-05	3.402E-02	35	N331	0 0 0 0 0	

4649. $C_{66}H_{84}O_{6}$
4-*tert*-Butylcalix[6]arene
5,11,17,23,29,35-Hexa-*tert*-butyl-37,38,39,40,41,42-hexahydroxycalix[6]arene
RN: 78092-53-2 **MP** (°C)**:** 380–381
MW: 973.40 **BP** (°C)**:** 890.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<9.73E-03	25	B424	1 0 1 2 2	

4650. $C_{66}H_{110}O_{55}$
6-*O*-α-D-Maltotriosyl-γ-cyclodextrin
6-*O*-α-Maltotriosyl-γ-cyclodextrin
RN: **MP** (°C)**:**
MW: 1783.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-01	1.516E+03	25	O321	0 0 0 0 0	
8.500E-01	1.516E+03	40	O321	0 0 0 0 0	
1.040E+00	1.855E+03	55	O321	0 0 0 0 0	

4651. $C_{67}H_{93}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-D-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1316.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.650E-04	4.806E-01	ns	B141	0 2 0 0 2	pH 7.5

4652. $C_{67}H_{93}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1316.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	4.937E-01	ns	B141	0 2 0 0 2	pH 7.5

4653. $C_{70}H_{89}N_{15}O_{13}$
Pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr
RN: **MP** (°C)**:**
MW: 1348.58 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-04	3.021E-01	ns	B141	0 2 0 0 2	pH 7.5

4654. $C_{70}H_{126}O_{35}$
β-Cyclodextrin, tetradeca-*O*-ethyl-
Heptakis(2,6-di-*O*-ethyl)-β-cyclodextrin
RN: 194715-43-0 **MP** (°C)**:**
MW: 1527.76 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.273E-05	5.000E-02	25	H319	0 0 0 0 0	

4655. $C_{72}H_{85}N_{19}O_{18}S_5$
Thiostrepton
Bryamycin
RN: 1393-48-2 **MP** (°C)**:** 210
MW: 1664.92 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-05	8.800E-02	21	M044	2 0 2 2 1	
1.442E-04	2.400E-01	28	A038	2 0 1 1 1	

4656. $C_{72}H_{100}N_{18}O_{17}PCo$
Coenzyme B12
Cobamamide
Cobalamin, Co-(5′-deoxy-5′-adenosyl)-
Dibencozide
Funacomide
Deoxyadenosylcobalamin
RN: 13870-90-1 **MP** (°C)**:**
MW: 1579.62 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-02	2.600E+01	24	M054	1 0 0 0 1	

4657. $C_{74}H_{100}ClN_{15}O_{14}$
Antarelix
AcDNal-Dcpa-ser-tyr-dhai-leu-lys(ipr)-pro-dala-NH2
RN: 151272-78-5 **MP** (°C)**:**
MW: 1459.17 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.85E-03	>1.00E+01	ns	D350	0 1 0 1 1	

4658. $C_{75}H_{122}N_{15}O_{46}S_{15}$
Pendecane(*S*-(carboxymethyl)-L-cysteine))
RN: **MP** (°C)**:**
MW: 2450.84 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-07	8.333E-04	25	N331	0 0 0 0 0	

4659. $C_{77}H_{107}N_{17}O_{15}$
Pro-pro-pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr
RN: **MP** (°C)**:**
MW: 1510.82 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-03	2.006E+00	ns	B141	0 2 0 0 2	pH 7.5

4660. $C_{80}H_{105}N_{17}O_{15}$

Pro-pro-pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr

RN: **MP** (°C)**:**

MW: 1544.83 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-04	1.298E+00	ns	B141	0 2 0 0 2	pH 7.5

4661. $C_{85}H_{117}N_{20}O_{18}$

Asp-arg-val-tyr-ile-his-pro-D-phe-his-leu-phe-val-tyr

RN: **MP** (°C)**:**

MW: 1707.00 **BP** (°C)**:**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-05	1.058E-01	20	B141	1 2 0 0 1	pH 7.5