

TABLE 1

Solute Name	$\Delta G(\text{kcal/mol})$	$\Delta S(\text{cal/mol}^\circ\text{K})$	$C_p(\text{cal/mol}^\circ\text{K})$
1_bromo.2_chloroethane	0.33(-1.95)	-19.73	239.39
1_bromo.2_methylpropane	0.99(-0.03)	-18.67	219.45
1_bromobutane	1.09(-0.40)	-23.40	264.57
1_bromoheptane	0.93(0.34)	-18.60	218.92
1_bromohexane	1.09(0.18)	-22.41	255.51
1_bromooctane	0.98(0.52)	-19.72	229.64
1_bromopentane	1.00(-0.10)	-19.91	231.83
1_bromopropane	0.93(-0.56)	-18.47	217.61
1_chloro.222_trifluoroethane	-0.41(0.06)	-25.65	309.97
1_chlorobutane	0.75(-0.16)	-17.44	201.54
1_chloroheptane	0.73(0.29)	-16.82	195.22
1_chlorohexane	0.99(0.00)	-25.60	278.88
1_chloropentane	0.64(-0.07)	-15.82	184.77
1_chloropropane	1.01(-0.33)	-23.57	264.02
1_ethylnaphthalene	-1.99(-2.40)	-25.25	158.07
1_iodobutane	-0.05(-0.25)	-22.60	240.17
1_iodoheptane	0.04(0.27)	-23.97	254.07
1_iodohexane	0.05(0.08)	-23.97	254.07
1_iodopentane	-0.01(-0.14)	-22.78	242.62
1_iodopropane	0.01(-0.53)	-24.55	258.48
1_methylimidazole	-4.86(-8.41)	-30.75	-120.71
1_methylpyrrole	-1.82(-2.89)	-19.73	77.68
1_methylcyclohexene	1.65(0.67)	-21.20	236.91
1_methylnaphthalene	-2.30(-2.44)	-18.70	98.62
1_naphthol	-8.45(-7.67)	-22.87	132.07
1_naphthylamine	-7.52(-7.28)	-28.22	233.37
1_nitrobutane	-0.57(-3.09)	-21.33	202.02
1_nitropentane	-0.72(-2.82)	-16.10	154.22
1_nitropropane	-0.55(-3.34)	-23.24	219.70
11_diacetoxyethane	-8.50(-4.97)	-32.95	-461.91
11_dichloroethane	0.25(-0.84)	-21.32	253.49
11_dichloroethene	1.12(0.25)	-18.86	243.35
11_diethoxyethane	-2.62(-3.28)	-30.73	-70.33
11_difluoroethane	-0.53(-0.11)	-21.69	225.05
111_trichloroethane	0.99(-0.19)	-20.97	255.51
111_trifluoro.222_trimethoxyethane	-3.16(-0.80)	-24.62	92.42
111_trifluoropropan.2_ol	-7.15(-4.16)	-27.88	287.08
111_trimethoxyethane	-3.98(-4.42)	-22.63	-171.60
1112_tetrachloroethane	0.37(-1.28)	-17.47	237.59
112_trichloro.122_trifluoroethane	1.75(1.77)	-19.52	244.16
112_trichloroethane	-1.15(-1.99)	-20.52	264.85
1122_tetrachloroethane	-0.34(-2.47)	-26.48	347.20
12_diacetoxyethane	-10.10(-6.34)	-33.51	-511.21
12_dibromoethane	0.72(-2.33)	-28.83	329.75

12_dichlorobenzene	-0.04(-1.36)	-22.76	265.02
12_dichloroethane	-0.87(-1.79)	-18.71	217.10
12_dichloropropane	-0.72(-1.27)	-17.77	198.38
12_diethoxyethane	-3.62(-3.54)	-24.71	-156.91
12_dimethoxyethane	-4.32(-4.84)	-31.93	-195.48
12_ethanediol	-12.26(-9.30)	-31.72	-125.58
123_trichlorobenzene	0.33(-1.24)	-21.99	274.80
123_trimethylbenzene	-0.31(-1.21)	-18.88	142.45
1234_tetrachlorobenzene	1.00(-1.34)	-26.08	320.25
1235_tetrachlorobenzene	1.11(-1.62)	-20.87	270.70
124_trichlorobenzene	0.69(-1.12)	-27.21	327.69
124_trimethylbenzene	-0.02(-0.86)	-26.24	212.85
1245_tetrachlorobenzene	1.13(-1.34)	-22.99	290.96
13_dichlorobenzene	0.06(-0.98)	-19.09	234.04
13_dichloropropane	-0.50(-1.89)	-18.52	201.92
13_dimethylnaphthalene	-2.02(-2.47)	-20.38	118.39
135_trichlorobenzene	0.84(-0.78)	-21.77	276.77
135_trimethylbenzene	-0.01(-0.90)	-25.43	208.56
14_dichlorobenzene	0.15(-1.01)	-23.36	274.19
14_dichlorobutane	-0.59(-2.32)	-23.90	245.02
14_dimethylpiperazine	-3.68(-7.58)	-28.18	-413.16
14_dimethylnaphthalene	-1.90(-2.82)	-24.79	161.12
14_dioxane	-3.43(-5.06)	-23.03	-112.85
2_bromo_2_methylpropane	0.59(0.84)	-16.92	186.52
2_bromopropane	0.92(-0.48)	-24.47	266.39
2_butoxyethanol	-4.54(-6.25)	-29.87	15.00
2_chloro_111_trimethoxyethane	-5.34(-4.59)	-26.17	-154.12
2_chloro_2_methylpropane	0.79(1.09)	-23.79	246.20
2_chloroaniline	-5.81(-4.91)	-20.61	263.27
2_chlorobutane	0.93(0.00)	-24.69	261.48
2_chlorophenol	-3.98(-4.55)	-21.44	228.36
2_chloropropane	0.73(-0.25)	-21.74	232.93
2_chloropyridine	-2.96(-4.39)	-29.14	71.02
2_chlorotoluene	-0.11(-1.14)	-23.66	239.96
2_ethoxyethanol	-9.56(-6.69)	-29.91	-248.54
2_ethylpyrazine	-5.11(-5.45)	-26.42	-150.68
2_ethylpyridine	-2.48(-4.33)	-27.22	-15.70
2_ethyltoluene	-0.19(-1.04)	-23.94	188.34
2_fluorophenol	-4.11(-5.29)	-23.80	249.78
2_iodophenol	-3.36(-6.20)	-22.83	251.70
2_iodopropane	-0.14(-0.46)	-23.50	237.59
2_isobutylpyrazine	-4.59(-5.04)	-26.86	-145.25
2_methoxy_111_trimethoxyethane	-7.81(-5.73)	-29.84	-429.85
2_methoxyaniline	-7.37(-6.12)	-25.53	132.39
2_methoxyethanamine	-6.77(-6.55)	-32.62	-164.08
2_methoxyethanol	-9.31(-6.76)	-30.93	-219.04
2_methoxyphenol	-5.84(-5.57)	-24.41	135.56
2_methyl_but_2_ene	1.61(1.31)	-19.92	226.79

2_methylbut_2_ene	1.56(1.31)	-18.36	211.84
2_methylbuta_13_diene	1.09(0.68)	-25.20	260.71
2_methylbutan_1_ol	-3.44(-4.42)	-25.64	56.31
2_methylbutan_2_ol	-2.86(-4.43)	-21.82	52.71
2_methylbutane	2.30(2.38)	-20.33	255.78
2_methylhexane	2.26(2.93)	-19.62	248.29
2_methylpent_1_ene	1.71(1.47)	-20.40	236.53
2_methylpentan_2_ol	-3.44(-3.92)	-20.69	16.24
2_methylpentan_3_ol	-2.19(-3.88)	-21.34	64.17
2_methylpentane	2.33(2.51)	-21.41	265.56
2_methylpropan_1_ol	-4.33(-4.50)	-23.88	108.93
2_methylpropan_2_ol	-3.48(-4.47)	-24.67	11.06
2_methylpropane	2.36(2.32)	-21.93	270.51
2_methylpropene	1.78(1.16)	-23.81	267.13
2_methylpyrazine	-5.46(-5.51)	-24.30	-172.01
2_methylpyridine	-2.80(-4.63)	-24.80	-69.26
2_methyltetrahydrofuran	-0.90(-3.30)	-21.10	18.85
2_methylthiophene	0.13(-1.38)	-24.82	237.70
2_naphthol	-8.36(-8.11)	-28.20	189.84
2_naphthylamine	-7.99(-7.47)	-24.23	186.15
2_nitroaniline	-6.14(-7.37)	-19.71	218.89
2_nitrophenol	-8.44(-4.58)	-19.69	234.31
2_nitropropane	-0.60(-3.13)	-22.61	204.45
2_nitrotoluene	-1.53(-3.58)	-20.76	191.05
2_phenylethanol	-6.69(-6.79)	-23.62	-16.04
2_propoxyethanol	-9.87(-6.40)	-27.76	-419.11
22_dimethylbutane	2.31(2.51)	-20.39	255.88
22_dimethylpentane	2.30(2.88)	-20.38	255.32
22_dimethylpropane	2.29(2.51)	-19.74	250.34
222_trifluoroethanol	-6.78(-4.31)	-26.35	301.40
224_trimethylpentane	2.34(2.89)	-21.61	267.67
225_trimethylhexane	2.36(2.93)	-22.43	275.19
23_dimethylbuta_13_diene	0.99(0.40)	-22.94	233.10
23_dimethylbutane	2.37(2.34)	-22.08	271.47
23_dimethylnaphthalene	-2.03(-2.78)	-20.40	118.38
23_dimethylpentane	2.24(2.52)	-18.71	239.60
23_dimethylphenol	-5.72(-6.16)	-20.09	171.33
23_dimethylpyridine	-2.72(-4.82)	-21.45	-99.29
234_trimethylpentane	2.26(2.56)	-19.28	245.41
24_dimethylpentan_3_one	-2.75(-2.74)	-25.03	-225.21
24_dimethylpentane	2.27(2.83)	-19.48	246.87
24_dimethylphenol	-5.66(-6.01)	-21.08	181.48
24_dimethylpyridine	-2.58(-4.86)	-27.03	-55.90
25_dimethylphenol	-3.78(-5.91)	-25.18	170.82
25_dimethylpyridine	-2.55(-4.72)	-24.82	-78.37
25_dimethyltetrahydrofuran	-0.58(-2.92)	-23.52	20.86
26_dimethylaniline	-4.58(-5.21)	-20.73	107.78
26_dimethylnaphthalene	-1.92(-2.63)	-23.71	149.16

26_dimethylphenol	-3.86(-5.26)	-24.48	176.84
26_dimethylpyridine	-2.34(-4.59)	-26.24	-42.48
3_acetylpyridine	-7.13(-8.26)	-30.53	-262.42
3_chloroaniline	-5.81(-5.82)	-22.19	301.13
3_chlorophenol	-5.64(-6.62)	-24.30	265.58
3_chloroprop_1_ene	0.29(-0.57)	-22.79	256.41
3_chloropyridine	-2.29(-4.01)	-23.84	47.99
3_cyanophenol	-8.40(-9.65)	-25.16	238.57
3_cyanopyridine	-4.84(-6.75)	-24.93	30.07
3_ethylphenol	-5.91(-6.25)	-23.58	181.25
3_ethylpyridine	-2.74(-4.59)	-23.93	-45.10
3_formylpyridine	-7.67(-7.10)	-26.18	-254.00
3_hydroxybenzaldehyde	-10.52(-9.50)	-21.59	-73.48
3_methoxyaniline	-8.25(-7.29)	-21.62	126.53
3_methoxyphenol	-8.14(-7.66)	-24.23	125.95
3_methyl_1h_indole	-6.13(-5.88)	-22.26	121.74
3_methyl_but_1_ene	1.87(1.83)	-23.07	267.51
3_methylbut_1_ene	1.83(1.82)	-21.90	256.24
3_methylbutan_1_ol	-5.47(-4.42)	-24.89	49.02
3_methylbutan_2_one	-3.20(-3.24)	-25.41	-162.96
3_methylbutanoic_acid	-8.72(-6.09)	-27.16	-26.63
3_methylheptane	2.32(2.97)	-21.54	267.13
3_methylhexane	2.39(2.71)	-22.98	280.73
3_methylpentane	2.28(2.51)	-19.77	249.59
3_methylpyridine	-2.83(-4.77)	-23.24	-50.57
3_nitroaniline	-7.88(-8.84)	-22.21	264.48
3_nitrophenol	-7.36(-9.62)	-21.72	281.97
3_nitrotoluene	-1.70(-3.45)	-21.61	197.29
3_phenylpropanol	-6.19(-6.92)	-29.46	38.02
33_dimethylbutan_2_one	-2.90(-3.11)	-28.01	-122.64
33_dimethylpentane	2.35(2.56)	-21.79	269.52
333_trimethoxypropionitrile	-7.15(-6.40)	-24.20	-97.24
34_dimethylphenol	-5.81(-6.50)	-23.23	182.87
34_dimethylpyridine	-2.70(-5.22)	-24.58	-45.67
35_dimethylphenol	-6.04(-6.27)	-24.58	192.76
35_dimethylpyridine	-2.50(-4.84)	-28.62	-36.09
4_acetylpyridine	-7.34(-7.62)	-27.64	-265.25
4_bromophenol	-6.18(-7.13)	-22.25	248.62
4_bromotoluene	-0.22(-1.39)	-22.80	231.63
4_chloro_3_methylphenol	-5.61(-6.79)	-23.66	251.34
4_chloroaniline	-6.31(-5.90)	-22.29	247.34
4_chlorophenol	-6.13(-7.03)	-21.95	238.03
4_cyanophenol	-8.71(-10.17)	-23.62	209.90
4_cyanopyridine	-4.99(-6.02)	-22.90	10.76
4_ethylphenol	-6.12(-6.13)	-24.98	196.15
4_ethylpyridine	-2.85(-4.73)	-25.25	-42.82
4_ethyltoluene	-0.12(-0.95)	-25.64	203.04
4_fluorophenol	-6.19(-6.19)	-21.20	226.04

4.formylpyridine	-7.49(-7.00)	-25.02	-215.11
4.hydroxybenzaldehyde	-11.45(-8.83)	-25.82	-77.79
4.isopropyltoluene	0.17(-0.68)	-27.00	236.90
4.methoxyacetophenone	-7.10(-4.40)	-30.71	-207.73
4.methoxyaniline	-8.16(-7.48)	-25.34	90.65
4.methyl_1h_imidazole	-7.65(-10.27)	-23.41	-220.78
4.methylacetophenone	-5.05(-4.70)	-29.32	-153.82
4.methylbenzaldehyde	-5.23(-4.27)	-26.83	-116.27
4.methylpentan_2.ol	-2.28(-3.73)	-23.57	174.63
4.methylpentan_2.one	-3.00(-3.05)	-26.60	-126.66
4.methylpyridine	-3.00(-4.93)	-23.31	-61.11
4.n.propylphenol	-6.02(-5.90)	-27.04	216.76
4.nitroaniline	-8.93(-10.27)	-23.36	289.36
4.nitrophenol	-7.78(-10.64)	-22.81	290.33
4.tert.butylphenol	-6.81(-5.91)	-29.81	195.45
acenaphthene	-2.24(-3.15)	-26.93	157.72
acetaldehyde	-4.03(-3.50)	-18.15	-125.51
acetic_acid	-9.69(-6.69)	-21.02	-111.71
acetonitrile	-2.32(-3.88)	-15.90	85.88
acetophenone	-5.24(-4.58)	-27.19	-167.65
alpha.methylstyrene	-1.00(-1.24)	-24.58	176.92
aniline	-6.56(-5.49)	-21.58	147.32
anisole	-2.45(-2.45)	-23.09	101.85
anthracene	-3.53(-3.95)	-29.15	170.54
azetidine	-3.49(-5.56)	-20.43	-180.12
benzaldehyde	-5.37(-4.02)	-24.61	-119.19
benzamide	-11.25(-11.00)	-28.34	-382.18
benzene	-0.66(-0.86)	-19.57	142.64
benzonitrile	-2.80(-4.21)	-22.11	143.25
benzotrifluoride	-1.39(-0.25)	-22.56	229.01
benzyl_alcohol	-5.93(-6.62)	-24.27	18.69
benzyl_bromide	-1.43(-2.38)	-23.09	197.06
benzyl_chloride	-1.59(-1.93)	-22.84	188.23
biphenyl	-2.11(-2.66)	-28.35	173.63
bis_2_chloroethyl_ether	-3.59(-4.23)	-24.27	128.88
bromobenzene	-0.44(-1.46)	-20.71	213.54
bromoethane	0.77(-0.74)	-16.39	198.11
bromomethane	0.74(-0.82)	-13.88	180.28
bromotrifluoromethane	1.49(1.79)	-15.80	211.29
but_1_ene	1.66(1.38)	-18.12	216.75
but_1_yne	0.99(-0.16)	-17.79	205.39
buta_1,3_diene	0.83(0.61)	-17.47	191.36
butan_1.ol	-4.20(-4.72)	-22.22	22.74
butan_2.ol	-3.34(-4.62)	-21.30	89.85
butanenitrile	-1.74(-3.64)	-20.35	121.06
butanoic_acid	-9.02(-6.35)	-25.30	-56.26
butanone	-3.67(-3.71)	-22.72	-123.34
butyraldehyde	-3.67(-3.18)	-22.72	-123.34

chlorobenzene	-0.36(-1.12)	-20.34	210.67
chlorodifluoromethane	-1.36(-0.50)	-14.28	256.61
chloroethane	0.57(-0.63)	-16.14	187.68
chloroethylene	0.64(-0.59)	-15.06	195.57
chlorofluoromethane	-0.95(-0.77)	-14.08	196.81
chloromethane	0.52(-0.55)	-13.56	171.11
cis_12_dimethylcyclohexane	2.39(1.58)	-23.01	281.17
cyanobenzene	-2.80(-4.10)	-22.11	143.25
cyclohepta_135_triene	-0.37(-0.99)	-21.31	166.59
cycloheptanol	-3.84(-5.48)	-25.14	23.30
cyclohexane	2.29(1.23)	-20.27	254.71
cyclohexanol	-4.40(-5.46)	-24.75	20.36
cyclohexanone	-3.36(-4.91)	-25.03	-160.43
cyclohexene	1.61(0.37)	-20.11	230.25
cyclohexylamine	-2.54(-4.59)	-22.94	109.27
cyclopentane	2.22(1.20)	-18.81	239.77
cyclopentanol	-4.33(-5.49)	-22.57	57.46
cyclopentanone	-3.26(-4.70)	-23.07	-126.20
cyclopentene	1.43(0.56)	-18.54	213.11
cyclopropane	1.97(0.75)	-15.49	205.42
decan_1_ol	-4.24(-3.64)	-35.11	154.87
decan_2_one	-2.81(-2.34)	-35.34	-16.28
di_isopropyl_sulfide	-0.15(-1.21)	-24.89	178.77
di_n_butyl_ether	0.20(-0.83)	-30.65	142.15
di_n_butylamine	-1.58(-3.24)	-32.26	3.71
di_n_propyl_ether	0.04(-1.16)	-26.52	102.26
di_n_propyl_sulfide	0.21(-1.28)	-26.08	226.91
di_n_propylamine	-1.71(-3.65)	-28.11	-33.60
dibromomethane	0.55(-1.96)	-15.59	217.61
dichloromethane	-0.03(-1.31)	-14.88	208.59
diethoxymethoxybenzene	-4.14(-5.23)	-35.53	46.36
diethyl_disulfide	-0.39(-1.64)	-23.82	222.21
diethyl_ether	-0.41(-1.59)	-22.43	46.02
diethyl_malonate	-9.08(-6.00)	-36.25	-384.68
diethyl_succinate	-8.07(-5.71)	-38.79	-417.40
diethyl_sulfide	-0.04(-1.46)	-21.91	181.04
diethylamine	-2.02(-4.07)	-23.98	-82.83
diiodomethane	-1.30(-2.49)	-16.65	244.51
diisopropyl_ether	0.31(-0.53)	-24.87	121.43
diisopropylamine	-1.33(-3.22)	-26.37	-6.79
dimethoxymethane	-2.25(-2.93)	-20.69	-38.37
dimethyl_disulfide	1.32(-1.83)	-18.25	223.16
dimethyl_ether	-1.15(-1.91)	-17.41	-12.30
dimethyl_sulfate	-8.76(-5.10)	-27.14	-372.40
dimethyl_sulfide	0.01(-1.61)	-16.73	161.70
dimethyl_sulfone	-10.82(-10.08)	-26.90	-629.28
dimethyl_sulfoxide	-7.92(-8.71)	-24.59	-496.79
dimethylamine	-3.72(-4.29)	-19.98	-184.32

E_12_dichloroethene	0.75(-0.78)	-16.44	226.42
E_but_2_enal	-4.67(-4.22)	-22.68	-175.96
E_hept_2_ene	1.86(1.68)	-24.81	280.26
E_hex_2_enal	-4.10(-3.68)	-26.68	-110.77
E_oct_2_enal	-3.85(-3.43)	-30.62	-47.53
ethanamide	-10.46(-9.71)	-22.48	-414.97
ethane	2.12(1.83)	-14.50	199.96
ethanethiol	-1.44(-1.14)	-16.61	181.74
ethanol	-5.03(-5.00)	-18.60	15.87
ethene	1.47(1.28)	-13.53	175.26
ethyl_acetate	-3.70(-2.94)	-24.79	-150.54
ethyl_benzoate	-4.81(-3.64)	-31.05	-171.77
ethyl_butanoate	-3.30(-2.49)	-29.35	-151.25
ethyl_formate	-3.83(-2.56)	-21.32	-88.21
ethyl_hexanoate	-3.19(-2.23)	-33.43	-101.25
ethyl_pentanoate	-3.40(-2.49)	-31.85	-176.80
ethyl_phenyl_ether	-2.00(-2.22)	-25.63	134.94
ethyl_propanoate	-3.63(-2.68)	-27.56	-197.38
ethylamine	-4.26(-4.50)	-19.55	-169.83
ethylbenzene	-0.33(-0.79)	-23.60	180.15
fluorene	-2.92(-3.35)	-28.38	163.51
fluorobenzene	-0.39(-0.80)	-19.55	203.10
fluoromethane	0.06(-0.22)	-12.86	141.41
formaldehyde	-4.25(-2.75)	-14.84	-91.50
halothane	0.20(-0.11)	-18.76	255.97
hept_1_ene	1.86(1.66)	-24.43	278.34
hept_1_yne	1.25(0.60)	-23.98	265.64
heptan_1_ol	-3.78(-4.21)	-28.46	77.61
heptan_2_one	-3.12(-3.04)	-29.57	-117.24
heptan_4_one	-2.75(-2.92)	-30.09	-176.66
heptanal	-3.27(-2.67)	-28.57	-32.32
hex_1_ene	1.79(1.58)	-22.32	258.71
hex_1_yne	1.16(0.29)	-21.91	245.96
hexa_15_diene	1.22(1.01)	-21.54	235.29
hexafluoropropene	0.64(-3.76)	-18.99	251.60
hexan_1_ol	-3.80(-4.40)	-26.52	33.19
hexan_2_one	-3.22(-3.28)	-27.50	-139.30
hexan_3_ol	-2.95(-4.06)	-25.03	128.96
hexanal	-3.46(-2.81)	-26.67	-61.24
hexanoic_acid	-8.67(-6.21)	-28.89	-48.15
hydrazine	-12.60(-9.30)	-18.51	-410.36
hydrogen_sulfide	-3.68(-0.70)	-10.40	209.39
imidazole	-7.74(-9.63)	-19.90	-143.44
indane	-0.41(-1.46)	-24.02	180.74
iodobenzene	-0.47(-1.74)	-21.14	229.63
iodoethane	-0.40(-0.74)	-17.22	189.51
iodomethane	-0.58(-0.89)	-14.71	178.18
isoamyl_acetate	-3.69(-2.21)	-30.65	-153.37

isoamyl_formate	-4.29(-2.13)	-27.35	-104.67
isobutyl_acetate	-3.36(-2.36)	-28.22	-102.85
isobutyl_formate	-3.89(-2.22)	-25.00	-45.38
isobutyl_isobutanoate	-2.70(-1.69)	-32.37	-116.13
isobutylbenzene	0.03(0.16)	-26.03	216.66
isobutyraldehyde	-3.42(-2.86)	-22.46	-131.92
isoflurane	-3.66(0.10)	-21.10	332.67
isopropyl_acetate	-3.50(-2.64)	-26.05	-134.21
isopropyl_formate	-3.42(-2.02)	-22.56	-40.95
isopropylbenzene	-0.25(-0.30)	-25.09	193.92
m_bis.trifluoromethyl_benzene	-2.67(1.07)	-24.71	263.08
m_cresol	-5.98(-5.49)	-22.95	177.45
m_xylene	-0.24(-0.83)	-23.65	187.04
methane	2.04(1.99)	-11.94	175.34
methanesulfonyl_chloride	-7.47(-4.87)	-21.62	-146.05
methanethiol	-1.44(-1.24)	-13.95	174.52
methanol	-5.45(-5.10)	-15.86	-22.58
methoxyflurane	-1.04(-1.12)	-21.55	202.05
methyl_acetate	-4.62(-3.13)	-22.97	-251.06
methyl_benzoate	-5.24(-3.92)	-28.63	-185.39
methyl_butanoate	-3.68(-2.83)	-26.74	-175.13
methyl_chloroacetate	-4.53(-4.00)	-22.45	-58.42
methyl_cyanoacetate	-7.00(-6.72)	-24.08	-91.59
methyl_cyclohexanecarboxylate	-3.04(-3.30)	-29.36	-139.70
methyl_cyclohexyl_ketone	-2.97(-3.90)	-28.29	-108.37
methyl_cyclopropanecarboxylate	-4.22(-4.10)	-26.20	-239.71
methyl_cyclopropyl_ketone	-3.01(-4.61)	-23.90	-126.95
methyl_ethyl_ether	-0.78(-2.10)	-19.88	22.43
methyl_ethyl_sulfide	-0.04(-1.50)	-19.31	172.16
methyl_formate	-4.07(-2.78)	-18.29	-67.18
methyl_hexanoate	-3.60(-2.49)	-30.87	-126.71
methyl_isopropyl_ether	-0.59(-2.01)	-21.37	30.21
methyl_methanesulfonate	-9.01(-4.87)	-26.53	-451.57
methyl_octanoate	-3.31(-2.04)	-34.83	-71.36
methyl_p_methoxybenzoate	-6.73(-5.33)	-31.92	-207.06
methyl_p_nitrobenzoate	-5.49(-6.88)	-29.54	-35.28
methyl_pentanoate	-3.79(-2.56)	-29.32	-204.79
methyl_propanoate	-4.06(-2.93)	-25.10	-233.78
methyl_propyl_ether	-0.77(-1.66)	-22.38	0.53
methyl_t_butyl_ether	-0.38(-2.21)	-22.55	53.54
methyl_tert_butyl_ether	-0.38(-2.21)	-22.55	53.39
methyl_trifluoroacetate	-2.64(-1.10)	-20.96	120.02
methyl_trimethylacetate	-3.15(-2.40)	-27.55	-154.69
methylamine	-5.02(-4.55)	-16.80	-171.59
methylcyclohexane	2.35(1.70)	-21.94	270.38
methylcyclopentane	2.28(1.59)	-20.56	257.17
morpholine	-5.20(-7.17)	-23.37	-235.89
N_acetylpyrrolidine	-6.74(-9.80)	-30.84	-573.75

n.butane	2.25(2.07)	-18.67	239.45
n.butanethiol	-1.21(-0.99)	-20.57	222.32
n.butylacetate	-3.79(-2.64)	-29.37	-148.75
n.butylacetamide	-9.73(-9.31)	-31.48	-412.56
n.butylamine	-4.31(-4.24)	-23.95	-160.52
n.butylbenzene	-0.21(-0.40)	-27.69	220.49
n.decane	2.63(3.16)	-31.16	358.88
n.heptane	2.44(2.67)	-24.91	299.31
n.heptylamine	-3.83(-3.79)	-29.50	-2.80
n.hexane	2.38(2.48)	-22.81	278.48
n.hexylacetate	-3.57(-2.26)	-33.29	-81.31
n.hexylamine	-3.86(-3.95)	-27.28	-46.53
n.hexylbenzene	-0.08(-0.04)	-31.83	259.72
N_methyl_N_222_trifluoroethyl_aniline	-4.90(-1.92)	-28.00	156.62
N_methylacetamide	-8.68(-10.00)	-25.90	-477.14
N_methylaniline	-5.38(-4.69)	-24.12	107.63
N_methylmorpholine	-3.66(-6.32)	-26.35	-332.36
N_methylpiperazine	-5.55(-7.77)	-28.67	-536.57
N_methylpiperidine	-1.28(-3.88)	-25.71	-213.10
n.nonane	2.57(3.13)	-29.06	338.15
n.octane	2.51(2.88)	-26.98	318.70
n.octylamine	-4.05(-3.65)	-32.07	-47.17
n.pentane	2.31(2.32)	-20.73	259.49
n.pentylacetate	-3.79(-2.51)	-31.61	-146.09
n.pentylpropanoate	-3.38(-2.11)	-34.09	-166.11
n.pentylamine	-4.48(-4.09)	-26.69	-219.31
n.pentylbenzene	-0.14(-0.23)	-29.81	241.23
n.pentylcyclopentane	2.53(2.55)	-28.46	332.42
n.propanethiol	-0.88(-1.06)	-16.67	1859.04
n.propylacetate	-3.72(-2.79)	-27.14	-152.61
n.propylbutyrate	-3.11(-2.28)	-31.46	-125.91
n.propylformate	-4.20(-2.48)	-23.70	-89.29
n.propylpropanoate	-3.46(-2.44)	-29.74	-183.94
n.propylamine	-4.13(-4.39)	-21.34	-115.49
n.propylbenzene	-0.23(-0.53)	-25.65	201.12
n.propylcyclopentane	2.40(2.13)	-24.34	292.99
naphthalene	-2.27(-2.40)	-24.46	150.35
nitrobenzene	-1.98(-4.12)	-21.46	200.22
nitroethane	-0.85(-3.71)	-17.61	168.93
nitromethane	-1.18(-4.02)	-15.20	159.58
NN_dimethyl_p_methylbenzamide	-7.89(-11.01)	-35.76	-451.94
NN_dimethyl_p_nitrobenzamide	-8.84(-9.76)	-35.29	-377.34
NN_dimethylaniline	-3.27(-11.95)	-26.30	16.89
NN_dimethylbenzamide	-8.20(-3.45)	-34.51	-555.70
NN_dimethylformamide	-6.53(-7.81)	-24.17	-388.31
non_1_ene	1.99(2.06)	-28.63	318.28
nonan_1_ol	-4.56(-3.88)	-33.87	122.18
nonan_2_one	-2.94(-2.49)	-33.54	-61.42

nonan_5_one	-2.56(-2.64)	-33.79	-84.91
nonanal	-3.25(-2.07)	-32.93	-2.65
o_cresol	-5.78(-5.87)	-22.58	194.64
o_toluidine	-5.68(-5.53)	-23.31	141.02
o_xylene	-0.29(-0.90)	-23.03	182.01
oct_1_ene	1.93(1.92)	-26.48	299.27
oct_1_yn	1.30(0.71)	-26.04	285.43
octan_1_ol	-5.21(-4.09)	-32.46	132.96
octan_2_ol	-3.02(-2.88)	-31.47	-79.84
octanal	-3.40(-2.29)	-30.98	-38.78
p_cresol	-6.27(-6.13)	-23.03	178.92
p_dibromobenzene	0.01(-2.30)	-22.07	261.95
p_toluidine	-6.28(-5.57)	-23.59	170.69
p_xylene	-0.26(-0.80)	-23.67	186.44
pent_1_ene	1.73(1.68)	-20.25	238.89
pent_1_yn	1.10(0.01)	-19.84	226.25
penta_1,4_diene	1.01(0.93)	-19.79	214.13
pentachloroethane	0.85(-1.39)	-20.52	279.26
pentan_1_ol	-3.89(-4.57)	-24.09	53.27
pentan_2_ol	-3.76(-4.39)	-23.98	78.55
pentan_2_ol	-3.29(-3.52)	-25.47	-163.37
pentan_3_ol	-3.35(-4.35)	-24.22	35.80
pentan_3_ol	-2.91(-3.41)	-25.31	-143.85
pentanal	-3.47(-3.03)	-24.63	-88.53
pentanenitrile	-1.67(-3.52)	-22.43	139.63
pentanoic_acid	-8.95(-6.16)	-27.16	-62.40
phenanthrene	-3.60(-3.88)	-28.83	170.17
phenol	-6.51(-6.61)	-20.98	157.77
phenyl_formate	-6.06(-3.82)	-25.24	-38.25
phenyl_methyl_sulfide	-1.25(-2.73)	-23.32	194.57
phenyl_trifluoroethyl_ether	-4.81(-1.29)	-26.28	236.32
piperazine	-6.72(-7.40)	-24.53	-291.42
piperidine	-2.42(-5.11)	-22.88	-54.99
prop_2_en_1_ol	-4.55(-5.03)	-19.15	41.35
propan_1_ol	-4.24(-4.85)	-19.63	18.10
propan_2_ol	-3.92(-4.74)	-20.42	-13.86
propane	2.18(1.96)	-16.60	219.71
propanenitrile	-1.91(-3.84)	-18.28	102.19
propanoic_acid	-9.75(-6.46)	-24.53	-131.96
propanone	-3.67(-3.80)	-20.89	-158.30
propene	1.53(1.32)	-16.02	195.54
propionaldehyde	-3.63(-3.43)	-20.30	-107.23
propyne	0.82(-0.48)	-15.46	183.20
pyrene	-4.36(-4.52)	-29.98	172.28
pyridine	-3.24(-4.69)	-21.26	-84.28
pyrrole	-4.40(-4.78)	-17.95	126.06
pyrrolidine	-3.19(-5.48)	-22.53	-204.41
quinoline	-3.93(-5.72)	-25.93	-44.46

sec_butylbenzene	-0.08(-0.45)	-26.64	216.12
styrene	-1.14(-1.24)	-22.90	165.57
teflurane	-0.49(0.50)	-17.92	264.28
tert_butylbenzene	-0.21(-0.44)	-26.15	200.65
tetrachloroethene	2.20(0.10)	-19.08	243.43
tetrachloromethane	2.07(0.08)	-17.80	230.53
tetrafluoromethane	1.42(3.12)	-14.53	201.16
tetrahydrofuran	-1.35(-3.47)	-20.44	-26.04
tetrahydropyran	-0.65(-3.12)	-21.45	43.55
thiophene	-0.29(-1.42)	-17.72	175.18
thiophenol	-2.41(-2.55)	-20.63	225.56
toluene	-0.46(-0.89)	-21.63	163.72
trans_14_dimethylcyclohexane	2.40(2.11)	-23.60	286.79
triacetyl_glycerol	-15.31(-8.84)	-36.02	-386.60
tribromomethane	1.19(-2.13)	-17.38	243.26
trichloroethene	1.13(-0.44)	-17.72	241.64
trichloromethane	0.38(-1.08)	-16.18	244.25
triethyl_phosphate	-10.74(-7.54)	-43.55	-1041.02
triethylamine	-0.44(-3.22)	-27.11	-131.58
trimethoxy_methane	-4.38(-4.42)	-25.24	-124.92
trimethoxymethylbenzene	-5.31(-4.04)	-34.02	-286.35
trimethyl_phosphate	-11.69(-8.70)	-34.87	-936.98
trimethylamine	-1.81(-3.20)	-22.18	-259.84
undecan_2_one	-3.05(-2.15)	-38.23	-65.23
Z_12_dichloroethene	-0.02(-1.17)	-16.31	221.63
Z_pent_2_ene	1.70(1.31)	-19.90	232.26