Environmental Organic Chemistry, 2nd Edition.
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Appendix C

Physicochemical Properties of Organic Compounds

Appendix C contains the names, molecular formula, molar mass (M_i), density (ρ_i), melting point (T_m), boiling point (T_b), vapor pressure (p_i^*), aqueous solubility (C_{iw}^{sat}), air–water partition constant (K_{iaw}), octanol–water partition constant (K_{iow}), and acidity constant (K_{ia}, where appropriate) of some environmentally relevant organic chemicals. Except for density (20°C), all data are given for 25°C. The data have been collected from various data compilations (and references cited therin) including Abraham et al. (1994a and b), Hansch et al. (1995), Lide (1998), Mackay et al. (1992-97), Mitchell and Jurs (1998), Montgomery (1997), and Ruelle and Kesselring (1997a and b).

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–log K_{iaw} calculated (experimental)	log K_{iow}	pK_{ia}
				n-Alkanes						
Methane	CH_4	16.0		–182.5	–164.0	7.45	2.82 (1bar)	–1.43	1.09	
Ethane	C_2H_6	30.1		–183.3	–88.6	6.61	2.69 (1bar)	–1.30	1.81	
Propane	C_3H_8	44.1		–189.7	–42.1	5.98	2.85 (1bar)	–1.46	2.36	
n-Butane	C_4H_{10}	58.1	0.58 (L)	–138.4	–0.5	5.40	2.98 (1bar)	–1.58	2.89	
n-Pentane	C_5H_{12}	72.2	0.63	–129.7	36.1	4.83	3.25	–1.69	3.39	
n-Hexane	C_6H_{14}	86.2	0.66	–95.0	69.0	4.30	3.83	–1.74	4.00	
n-Heptane	C_7H_{16}	100.2	0.68	–90.6	98.4	3.79	4.53	–1.93	4.66	
n-Octane	C_8H_{18}	114.2	0.70	–56.8	125.7	3.26	5.20	–2.07	5.15	
n-Nonane	C_9H_{20}	128.3	0.72	–51.0	150.8	2.76	5.77	–2.14	5.65	
n-Decane	$C_{10}H_{22}$	142.3	0.73	–29.7	174.1	2.24	6.42	–2.27	6.25	
n-Undecane	$C_{11}H_{24}$	156.3	0.74	–25.6	195.9	1.72				
n-Dodecane	$C_{12}H_{26}$	170.3	0.75	–9.6	216.3	1.19	7.52	–2.32		
n-Hexadecane	$C_{16}H_{34}$	226.4	0.77	18.2	287.0	–0.73	7.80	–0.68		
n-Octadecane	$C_{18}H_{38}$	254.4	0.78	28.2	316.1	–1.78	8.08	–0.09		
				Branched Alkanes						
2-Methylpropane (isobutane)	C_4H_{10}	58.1	0.56 (L)	–159.4	–11.7	5.56	3.07 (1bar)	–1.68	2.82	
2-Methylbutane (isopentane)	C_5H_{12}	72.2	0.62	–159.9	27.9	4.96	3.18	–1.75		
2,2-Dimethylpropane (neopentane)	C_5H_{12}	72.2	0.59 (L)	–16.6	9.5	5.24	3.34 (1bar)	–1.95	3.11	
2-Methylpentane (isohexane)	C_6H_{14}	86.2	0.64	–153.8	60.1	4.45	3.80	–1.86	3.60	
2,2-Dimethylbutane (neohexane)	C_6H_{14}	86.2	0.65	–99.8	49.7	4.63	3.65	–1.89	3.42	
2,2,4-Trimethylpentane (isooctane)	C_8H_{18}	114.2	0.69	–107.4	99.2	3.81	4.67	–2.09		
				Unsaturated and Alicyclic Hydrocarbons						
1.3-Butadiene	C_4H_6	54.1	0.62 (L)	–108.9	–4.4	5.45	1.86	–0.47	1.99	
2-Methyl-1,3-butadiene (isoprene)	C_5H_8	68.1	0.68	–146.0	34.0	4.86	2.04	–0.51	2.05	
1,4-Pentadiene	C_5H_8	68.1	0.66	–148.3	26.0	5.00	2.08	–0.69		
Cyclopentene	C_5H_8	68.1	0.77	–135.1	44.2	4.70	2.09	–0.40		
Cyclopentane	C_5H_{10}	70.1	0.74	–92.9	49.2	4.63	2.64	–0.88	3.00	
1,4-Cyclohexadiene	C_6H_8	80.1	0.85	–49.2	81.5	3.95	2.03	0.41	2.30	
Cyclohexene	C_6H_{10}	82.1	0.81	–103.5	83.0	4.07	2.60	–0.28	2.86	
Cyclohexane	C_6H_{12}	84.2	0.78	6.5	80.7	4.10	3.17	–0.89	3.44	
1-Hexene	C_6H_{12}	84.2	0.67	–139.8	63.4	4.40	3.22	–1.22	3.40	
Methylcyclohexane	C_7H_{14}	98.2	0.77	–126.6	100.6	3.79	3.81	–1.21	3.88	

				Alkylated Benzenes					
Benzene	C_6H_6	78.1	0.88	5.5	80.1	4.10	1.65	0.65 (0.65 exp.)	2.17
Methylbenzene (toluene)	C_7H_8	92.2	0.87	–95.0	110.6	3.57	2.22	0.60 (0.62 exp.)	2.69
Ethylbenzene	C_8H_{10}	106.2	0.86	–95.0	136.2	3.09	2.80	0.50 (0.47 exp.)	3.20
Vinylbenzene (styrene)	C_8H_8	104.2	0.91	–31.0	145.1	2.94	2.53	0.93 (0.92 exp.)	2.95
1,2-Dimethylbenzene (*o*-xylene)	C_8H_{10}	106.2	0.88	–25.2	144.4	2.95	2.75	0.69 (0.68 exp.)	3.16
1,3-Dimethylbenzene (*m*-xylene)	C_8H_{10}	106.2	0.86	–47.8	139.1	3.04	2.82	0.53 (0.52 exp.)	3.30
1,4-Dimethylbenzene (*p*-xylene)	C_8H_{10}	106.2	0.86	13.3	138.1	3.07	2.77	0.55 (0.54 exp.)	3.27
n-Propylbenzene	C_9H_{12}	120.2	0.86	–99.6	159.2	2.65	3.34	0.40	3.69
Isopropylbenzene	C_9H_{12}	120.2	0.86	–96.6	154.2	2.79	3.33	0.27	3.66
1,2,3-Trimethylbenzene	C_9H_{12}	120.2	0.89	–25.4	176.1	2.30	3.23	0.86	3.60
1,2,4-Trimethylbenzene	C_9H_{12}	120.2	0.88	–43.8	169.4	2.42	3.33	0.65	3.65
1,3,5-Trimethylbenzene	C_9H_{12}	120.2	0.88	–44.7	164.7	2.52	3.38	0.50	3.42
1-Ethyl-2-methylbenzene	C_9H_{12}	120.2	0.88	–83.8	165.2	2.52	3.20	0.67	3.53
1-Ethyl-4-methylbenzene	C_9H_{12}	120.2	0.86	–62.4	162.0	2.60	3.10	0.69	3.63
n-Butylbenzene	$C_{10}H_{14}$	134.2	0.86	–88.0	183.0	2.15	3.95	0.29	4.38
s-Butylbenzene	$C_{10}H_{14}$	134.2	0.86	–75.0	174.0	2.40	3.73	0.26	4.44
t-Butylbenzene	$C_{10}H_{14}$	134.2	0.87	–58.0	169.0	2.46	3.60	0.33	4.11
1,2,3,4-Tetramethylbenzene	$C_{10}H_{14}$	134.2	0.91	–6.3	205.0	1.65			4.00
1,2,4,5-Tetramethylbenzene	$C_{10}H_{14}$	134.2	0.84	79.5	195.9	1.11	4.58	0.70	4.10
n-Pentylbenzene	$C_{11}H_{16}$	148.3	0.86	–78.3	202.2	1.65	4.59	0.15	4.90
n-Hexylbenzene	$C_{12}H_{18}$	162.3	0.86	–61.0	226.0	1.13	5.20	0.06	5.52
Hexamethylbenzene	$C_{12}H_{18}$	162.3		166.7	265.0	–0.80	5.84	1.35	4.75
				Polycyclic Aromatic Hydrocarbons and Related Compounds					
Indane	C_9H_{10}	118.2	0.96	–51.4	178.0	2.30	3.03	1.06	3.33
Naphthalene	$C_{10}H_8$	128.2	1.16	80.2	218.0	1.05	3.60	1.74 (1.72 exp.)	3.33
1-Methylnaphthalene	$C_{11}H_{10}$	142.2	1.02	–22.0	244.0	0.92	3.71	1.76	3.87
2-Methylnaphthalene	$C_{11}H_{10}$	142.2	1.01	35.0	241.0	0.95	3.75	1.69	3.99
Acenaphthene	$C_{12}H_{10}$	154.2	1.05	96.2	278.0	–0.51	4.61	2.29 (2.28 exp.)	4.20
Acenaphthylene	$C_{12}H_8$	152.2	0.90	92.5	270.0	–0.05	4.59	1.85	4.00
Fluorene	$C_{13}H_{10}$	166.2	1.20	116.0	295.0	–1.02	4.94	2.47 (2.39 exp.)	4.32

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–log K_{iaw} calculated (experimental)	log K_{iow}	pK_{ia}
Phenanthrene	$C_{14}H_{10}$	178.2	0.98	101.0	339.0	–1.66	5.20	2.85 (2.93 exp.)	4.57	
Anthracene	$C_{14}H_{10}$	178.2	1.25	217.5	341.0	–3.01	6.60	2.80 (2.77 exp.)	4.68	
Fluoranthene	$C_{16}H_{10}$	202.3	1.25	110.5	384.0	-2.91	5.96	3.34 (3.35 exp.)	5.23	
Pyrene	$C_{16}H_{10}$	202.3	1.27	156.0	403.0	–3.09	6.16	3.32 (3.36 exp.)	5.13	
Benzo(a)anthracene	$C_{18}H_{12}$	228.3	1.25	160.6	437.5	–4.60	7.32	3.68	5.91	
Chrysene	$C_{18}H_{12}$	228.3	1.28	255.0	448.0	–6.22	8.05	4.56	5.81	
Benzo(a)pyrene	$C_{20}H_{12}$	252.3		176.5	496.0	–6.15	8.14	4.79 (4.86 exp.)	6.13	
Perylene	$C_{20}H_{12}$	252.3		277.0	503.0	–7.85	8.80	5.44	6.25	
Chlorinated C_1- to C_4-Compounds										
Chloromethane	CH_3Cl	50.5	0.92 (L)	–97.7	–24.2	5.76	0.98 (1bar)	0.42	0.91	
Dichloromethane	CH_2Cl_2	84.9	1.33	–95.1	40.1	4.76	0.70	0.93 (0.97 exp.)	1.31	
Trichloromethane	$CHCl_3$	119.4	1.48	–63.3	61.4	4.40	1.15	0.84 (0.82 exp.)	1.95	
Tetrachloromethane	CCl_4	153.8	1.59	—23.0	76.7	4.16	2.27	–0.04 (0.05 exp.)	2.77	
1,1–Dichloroethane	$C_2H_4Cl_2$	99.0	1.18	–97.3	57.3	4.49	1.29	0.61 (0.62 exp.)	1.79	
1,2-Dichloroethane	$C_2H_4Cl_2$	99.0	1.25	–35.5	83.6	4.05	1.07	1.27 (1.30 exp.)	1.46	
1,1,1-Trichloroethane	$C_2H_3Cl_3$	133.4	1.34	–31.4	73.9	4.22	2.01	–0.16 (0.15 exp.)	2.49	
1,1,2-Trichloroethane	$C_2H_3Cl_3$	133.4	1.44	–37.0	113.6	3.60	1.47	1.32 (1.40 exp.)	2.34	
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	167.9	1.60	–40.8	146.3	2.90	1.71	1.78 (1.85 exp.)	2.39	
Pentachloroethane	C_2HCl_5	202.3	1.68	–29.0	160.8	2.79	2.61	0.99	3.22	
Hexachloroethane	C_2Cl_6	236.7	2.09	187.5	187.5	1.70	3.68	1.01	3.93	
Chloroethene	C_2H_3Cl	62.5	0.91 (L)	–153.8	–13.7	5.55	1.35 (1bar)	–0.04 (–0.05 exp.)	1.27	
1,1-Dichloroethene	$C_2H_2Cl_2$	96.9	1.22	–122.0	31.7	4.90	1.59	–0.10 (–0.03 exp.)	1.48	
cis-1,2-Dichloroethene	$C_2H_2Cl_2$	96.9	1.27	–81.0	60.0	4.45	1.28	0.66 (0.79 exp.)	1.86	
trans-1,2-Dichloroethene	$C_2H_2Cl_2$	96.9	1.27	–50.0	48.0	4.61	1.19	0.59 (0.46 exp.)	2.09	

Trichloroethene	C_2HCl_3	131.4	1.46	–73.0	87.0	4.00	2.08	0.31 (0.40 exp.)	2.42
Tetrachloroethene	C_2Cl_4	165.8	1.62	–22.4	121.1	3.40	3.07	–0.08 (0.12 exp.)	2.88
3-Chloro-1-propene	C_3H_5Cl	76.5	0.94	–135.0	44.9	4.70	1.33	0.36 (0.42 exp.)	1.45
Brominated and Iodated C_1- and C_2-Compound									
Bromomethane	CH_3Br	94.9	1.68 (L)	–93.6	3.6	5.34	0.79 (1bar)	0.35	1.19
Dibromomethane	CH_2Br_2	173.9	2.50	–52.6	96.7	3.81	1.18	1.40 (1.20 exp.)	1.88
Tribromomethane	$CHBr_3$	252.8	2.89	8.3	149.6	2.86	1.91	1.62 (1.72 exp.)	2.67
Bromoethane	C_2H_5Br	109.0	1.45	–119.0	38.4	4.80	1.09	1.50	1.61
1,2-Dibromoethane	$C_2H_4Br_2$	187.9	2.18	9.8	131.5	3.21	1.63	1.55	1.96
Bromoethene	C_2H_3Br	107.0	1.49 (L)	–139.5	15.8	5.15			1.57
Iodomethane	CH_3I	141.9	2.28	–66.5	42.5	4.73	1.01	0.66 (0.65 exp.)	1.51
Iodoethane	C_2H_5I	156.0	1.94	–111.0	72.4	4.26	1.60	0.53	2.00
Mixed Halogenated C_1– and C_2-Compounds									
Bromochloromethane	CH_2BrCl	129.4	1.93	–88.0	68.1	4.29	0.94	1.16	1.41
Bromodichloromethane	$CHBrCl_2$	163.8	1.97	–57.1	90.0	3.82	1.55	1.01	2.10
Dichlorodifluoromethane (Freon 12)	CCl_2F_2	120.9	1.33 (L)	–158.0	–29.8	5.75	2.64 (1bar)	–1.25 (–1.18 exp.)	2.16
Trichlorofluoromethane (Freon 11)	CCl_3F	137.4	1.18	–111.0	23.8	5.03	2.10 (1bar)	–0.71 (–0.61 exp.)	2.53
1,1,2-Trichloro-1,2,2-trifluoroethane (Freon 113)	$C_2Cl_3F_3$	187.4	1.57	–35.0	47.6	4.68	3.04	–1.29 (–1.11 exp.)	3.16
1,1,2,2-Tetrachloro-1,2-difluoroethane (Freon 112)	$C_2Cl_4F_2$	203.8	1.64	–25.5	92.8	3.87	3.23	–0.71	3.73
Chlorobenzenes									
Chlorobenzene	C_6H_5Cl	112.6	1.11	-45.2	132.0	3.20	2.39	0.80 (0.82 exp.)	2.78
1,2-Dichlorobenzene	$C_6H_4Cl_2$	147.0	1.30	–17.0	180.0	2.30	3.05	1.04 (1.00 exp.)	3.40
1,3-Dichlorobenzene	$C_6H_4Cl_2$	147.0	1.29	–24.7	173.0	2.45	3.08	0.86 (0.82 exp.)	3.47
1,4-Dichlorobenzene	$C_6H_4Cl_2$	147.0	1.25	53.1	174.0	2.05	3.30	1.04 (1.10 exp.)	3.45
1,2,3-Trichlorobenzene	$C_6H_3Cl_3$	181.5	1.69	52.0	218.5	1.45	3.94	1.01	4.14
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	181.5	1.45	17.0	213.5	1.58	3.78	1.03	4.06
1,3,5-Trichlorobenzene	$C_6H_3Cl_3$	181.5	1.39	63.5	208.0	1.50	4.53	0.36	4.19

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–log K_{iaw} calculated (experimental)	log K_{iow}	pK_{ia}
1,2,3,4-Tetrachlorobenzene	$C_6H_2Cl_4$	215.9		47.5	254.0	0.75	4.69	0.95	4.64	
1,2,3,5-Tetrachlorobenzene	$C_6H_2Cl_4$	215.9	1.86	54.5	246.0	1.00	4.79	0.60	4.66	
1,2,4,5-Tetrachlorobenzene	$C_6H_2Cl_4$	215.9		140.0	243.0	–0.14	5.23	1.30	4.72	
Pentachlorobenzene	C_6HCl_5	250.3	1.83	86.0	277.0	–0.66	5.58	1.47	5.18	
Hexachlorobenzene	C_6Cl_6	284.8	2.08	230.0	322.0	–2.60	7.55	1.44 (1.54 exp.)	5.80	
Polychlorinated Biphenyls (PCBs), Selected Congeners										
Biphenyl	$C_{12}H_{10}$	154.2	0.87	71.0	255.9	0.11	4.34	1.93	4.01	
2-CBP (PCB1)	$C_{12}H_9Cl$	188.6	0.98	34.0	274.0	–0.30	4.54	1.55	4.53	
4-CBP (PCB3)	$C_{12}H_9Cl$	188.6	0.98	77.7	291.0	–0.57	5.19	1.77	4.61	
2,2'-CBP (PCB4)	$C_{12}H_8Cl_2$	223.1	1.05	61.0		–0.58	5.35	1.62	4.97	
2,4-CBP (PCB7)	$C_{12}H_8Cl_2$	223.1	1.05	24.4		–0.60	5.25	1.74	5.30	
2,4'-CBP (PCB8)	$C_{12}H_8Cl_2$	223.1	1.05	45.0		–1.10	5.35	2.14	5.10	
4,4'-CBP (PCB15)	$C_{12}H_8Cl_2$	223.1	1.05	148.5		–2.30	6.57	2.12	5.33	
2,2',5-CBP (PCB18)	$C_{12}H_7Cl_3$	257.5	1.15	44.0		–0.84	5.80	1.43	5.60	
2,4,4'-CBP (PCB28)	$C_{12}H_7Cl_3$	257.5	1.15	57.5		–1.70	6.20	1.89	5.62	
2,4,5-CBP (PCB29)	$C_{12}H_7Cl_3$	257.5	1.15	78.5		–1.95	6.26	2.08	5.90	
2,2',4,4'-CBP (PCB47)	$C_{12}H_6Cl_4$	292.0	1.20	41.5		–2.00	6.51	1.88	6.29	
2,2',5,5'-CBP (PCB52)	$C_{12}H_6Cl_4$	292.0	1.20	86.5		–2.30	6.99	1.70	6.09	
3,3',4,4'-CBP (PCB77)	$C_{12}H_6Cl_4$	292.0	1.20	180.0			7.47		6.50	
2,2',3,4,5'-CBP (PCB87)	$C_{12}H_5Cl_5$	326.4	1.28	112.0		–3.52	7.91	2.00	6.37	
2,2',4,5,5'-CBP (PCB101)	$C_{12}H_5Cl_5$	326.4	1.28	77.0		–2.96	7.51	1.83	6.36	
2,2',4,4',5,5'-CBP (PCB153)	$C_{12}H_4Cl_6$	360.9		103.5		–3.92	8.55	1.76	7.15	
2,2',3,4,4',5,5'-CBP (PCB180)	$C_{12}H_3Cl_7$	395.4		109.5				2.36	7.36	
Miscellanous Polychlorinated Compounds										
α-hexachlorocyclohexane (α-HCH)	$C_6H_6Cl_6$	290.8		158.0		–2.52	5.28	3.63	3.81	
β-hexachlorocyclohexane (β-HCH)	$C_6H_6Cl_6$	290.8		309.5		–4.40	6.46	4.33	3.80	
γ-hexachlorocyclohexane (lindane, γ-HCH)	$C_6H_6Cl_6$	290.8		112.0		–2.15	4.60	3.94	3.78	
p,p'-DDT	$C_{14}H_9Cl_5$	354.5	1.55	109.0		–4.70	7.80	3.30	6.36	
p,p'-DDE	$C_{14}H_8Cl_4$	318.0		89.0		–3.20	6.90	2.69	5.70	
p,p'-DDD	$C_{14}H_{10}Cl_4$	320.0		109.5		–3.90	6.80	3.49	5.50	

				Aliphatic Ethers					
Dimethyl ether	C_2H_6O	46.1	0.67	−141.5	−24.8	5.77		(1.40 exp.)	0.10
Diethyl ether	$C_4H_{10}O$	74.1	0.71	−116.3	34.5	4.85	0.05	1.49	0.89
Methyl-*t*-butyl-ether (MBTE)	$C_5H_{12}O$	88.2	0.74	−109.0	55.2	4.51	0.34	1.54	0.94
Di-*n*-propyl ether	$C_6H_{14}O$	102.2	0.75	−123.2	90.1	3.92	1.50	0.97	2.03
Di-isopropyl ether	$C_6H_{14}O$	102.2	0.73	−85.5	68.5	4.30	1.10	0.98	1.52
n-Butyl-ethyl ether	$C_6H_{14}O$	102.2	0.75	−103.0	92.2	3.90	1.20	1.29	2.03
D-*n*-butyl ether	$C_8H_{18}O$	130.2	0.77	−95.2	140.3	2.95	2.75	0.69	3.21
				Miscellaneous Ethers Including Epoxides					
Ethylene oxide (epoxyethane)	C_2H_4O	44.1	0.87	−111.0	10.7	5.16	−0.93 (1bar)		−0.30
Propyleneoxide (epoxypropane)	C_3H_6O	58.1	0.83	−112.1	34.2	4.85	−0.91		0.03
Tetrahydrofuran	C_4H_8O	72.1	0.89	−108.5	66.0	4.33	miscible	(2.55 exp.)	0.46
1,4-Dioxane	$C_4H_8O_2$	88.1	1.03	11.0	101.1	3.70	miscible	(3.71 exp.)	−0.27
1-Chloro-2,3-epoxypropane (epichlorohydrine)	C_3H_5ClO	92.5	1.18	−57.2	116.2	3.36	0.15	2.88	0.30
Di-2-chloroethyl ether	$C_4H_8Cl_2O$	143.0	1.22	−46.8	178.0	2.31	1.15	2.93	1.29
Methoxybenzene (anisole)	C_7H_8O	108.2	0.99	−37.5	153.6	2.67	1.80	1.92	2.11
Ethoxybenzene (phenetole)	$C_8H_{10}O$	122.2	1.07	−31.0	169.5	2.31	2.18	1.90	2.51
Styreneoxide	C_8H_8O	120.2	1.05	−35.6	194.1	1.60	1.63	3.16	1.55
				Polychlorinated Dibenzo-p-Dioxins (PCDDs), Selected Congeners					
Dibenzo-*p*-dioxin (DD)	$C_{12}H_8O_2$	184.0		123.0	283.5	−1.26	5.33	2.32	4.30
1-CDD	$C_{12}H_7ClO_2$	218.5		105.5	315.5	−1.92	5.72	2.59	4.90
2,7-DCDD	$C_{12}H_6Cl_2O_2$	253.0		210.0	373.5	−3.92	7.83	2.48	5.70
1,2,3,4-TCDD	$C_{12}H_4Cl_4O_2$	322.0		190.0	419.0	−5.20	8.77	2.82	6.60
2,3,7,8-TCDD	$C_{12}H_4Cl_4O_2$	322.0		305.0	446.5	−6.70	10.22	2.87	6.80
1,2,3,4,7-PCDD	$C_{12}H_3Cl_5O_2$	356.4		196.0	464.7	−7.05	9.48	3.96	7.40
1,2,3,4,7,8-HCDD	$C_{12}H_2Cl_6O_2$	391.0		273.0	487.7	−8.29	10.94	3.74	7.80
Octachloro-DD	$C_{12}Cl_8O_2$	460.0		322.0	510.0	−10.00	12.79	3.60	8.20
				Polychlorinated Dibenzofurans (PCDFs), Selected Congeners					
Dibenzofuran (DF)	$C_{12}H_8O$	168.2		86.5	287.0	−0.52	4.55	2.36	4.31
2,8-DCDF	$C_{12}H_6Cl_2O$	237.1		184.0	375.0	−3.41	7.21	2.59	5.44
2,3,7,8-TCDF	$C_{12}H_4Cl_4O$	306.0		227.0	438.0	−5.70	8.86	3.23	6.10
2,3,4,7,8-PCDF	$C_{12}H_3Cl_5O$	340.4		196.0	464.7	−6.46	9.16	3.87	6.50
1,2,3,4,7,8-HCDF	$C_{12}H_2Cl_6O$	374.9		225.5	487.7	−7.50	10.66	3.23	7.00
Octachloro-DF	$C_{12}Cl_8O_2$	443.8		258.0	537.0	−9.30	11.58	4.11	8.00

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–logK_{iaw} calculated (experimental)	logK_{iow}	pK_{ia}
				Alkylated Phenols						
Phenol	C_6H_6O	94.1	1.05	40.9	181.8	1.79	0.005	4.59 (4.79 exp.)	1.44	9.95
2-Methylphenol (*o*-cresol)	C_7H_8O	108.1	1.05	30.7	191.0	1.60	0.61	4.18 (4.30 exp.)	2.07	10.28
3-Methylphenol (*m*-cresol)	C_7H_8O	108.1	1.03	11.9	202.1	1.30	0.67	4.42	1.98	10.05
4-Methylphenol (*p*-cresol)	C_7H_8O	108.1	1.03	35.2	201.9	1.20	0.75	4.44 (4.49 exp.)	1.93	10.25
4-Ethylphenol	$C_8H_{10}O$	122.2	1.03	47.0	219.0	0.80	1.18	4.40	2.50	10.00
2,6-Dimethylphenol	$C_8H_{10}O$	122.2	1.13	49.0	203.0	1.28	1.29	3.70 (3.56 exp.)	2.36	10.63
3,4-Dimethylphenol	$C_8H_{10}O$	122.2	1.14	67.0		–0.07	1.40	5.06	2.23	10.34
2,4,6-Trimethylphenol	$C_9H_{12}O$	136.2		72.0		0.82	2.10	3.47	2.73	10.90
4-*n*-Butylphenol	$C_{10}H_{14}O$	150.2	0.98	22.0	248.0		2.31		3.64	
4-*t*-Butylphenol	$C_{10}H_{14}O$	150.2		99.0	238.0	0.08	2.11	4.20	3.14	9.90
4-*n*-Octylphenol	$C_{14}H_{22}O$	206.3		41.5		–1.14	4.18	3.35		
4-*n*-Nonylphenol	$C_{15}H_{24}O$	220.4	1.51	96.0	295.0	–1.15	4.64	2.89	5.76	
				Chlorinated Phenols						
2-Chlorophenol	C_6H_5ClO	128.6	1.26	9.8	175.2	2.50	0.65	3.24	2.19	8.44
3-Chlorophenol	C_6H_5ClO	128.6	1.25	32.6	214.0	1.54	0.69	4.16	2.48	8.98
4-Chlorophenol	C_6H_5ClO	128.6	1.31	42.7	219.0	1.27	0.68	4.43	2.42	9.29
2,4-Dichlorophenol	$C_6H_4Cl_2O$	163.0	1.38	43.7	213.0	1.20	1.57	3.61	3.09	7.85
2,4,5-Trichlorophenol	$C_6H_3Cl_3O$	197.5	1.50	62.5		0.62	2.22	3.55	3.90	6.91
2,4,6-Trichlorophenol	$C_6H_3Cl_3O$	197.5		68.8	243.5	0.37	2.37	3.65	3.67	6.19
2,3,4,5-Tetrachlorophenol	$C_6H_2Cl_4O$	231.9		117.0		–1.00	3.15	4.24	4.87	6.35
2,3,4,6-Tetrachlorophenol	$C_6H_2Cl_4O$	231.9		69.5		–0.55	3.10	3.84	4.45	5.40
Pentachlorophenol	C_6HCl_5O	266.3		189.3		–2.04	4.15	4.28	5.24	4.83
				Nitrophenols						
2-Nitrophenol	$C_6H_5NO_3$	139.1	1.55	44.7	215.0	1.26	2.03	3.10 (3.40 exp.)	1.78	7.15
3-Nitrophenol	$C_6H_5NO_3$	139.1		96.5			1.03		2.00	8.36
4-Nitrophenol	$C_6H_5NO_3$	139.1	1.48	114.0		–2.26	0.98	7.66	1.96	7.06
2,4-Dinitrophenol	$C_6H_4N_2O_5$	184.1		114.1			2.74		1.66	4.01
2,4-Dinitro-6-methylphenol (dinitro-*o*-cresol; DNOC)	$C_7H_6N_2O_5$	198.1		86.5		–1.14	3.00	4.53	2.12	4.31

				Miscellaneous Phenolic Compounds						
1,2-Dihydroxybenzene (catechol)	$C_6H_6O_2$	110.1	1.15	104.0	245.0	−0.65	0.39	(6.65)	0.88	9.34 12.60
1,3-Dihydroxybenzene (resorcinol)	$C_6H_6O_2$	110.1	1.27	110.0	277.0	−2.93	0.00	(9.32)	0.80	9.32 11.10
1,4-Dihydroxybenzene (*hydroquinone*)	$C_6H_6O_2$	110.1	1.33	172.0	287.0	−2.59	0.20	(8.78)	0.59	9.85 11.40
2-Methoxyphenol (guaiacol)	$C_7H_8O_2$	124.1		32.0	205.0	1.32	0.70	4.38 (4.28 exp.)	1.32	
4,5-Dichloro-2-methoxyphenol (4,5-dichloroguaiacol)	$C_7H_6Cl_2O_2$	193.0		74.0		−0.24	2.52	4.11	3.26	8.52
3,4,5-trichloro-2-methoxyphenol (3,4,5-Trichloro-guaiacol)	$C_7H_5Cl_3O_2$	227.5		85.5		−0.79	2.86	4.32	3.77	7.56
4,5,6-Trichloro-2-methoxyphenol (4,5,6-trichloro-guaiacol)	$C_7H_5Cl_3O_2$	227.5		113.5		−1.49	3.62	4.26	3.74	7.07
Tetrachloro-2-methoxyphenol (tetrachloroguaicol)	$C_7H_4Cl_4O_2$	261.9		121.5		−1.80	4.00	4.19	4.45	6.26
				Aldehydes						
Methanal (formaldehyde)	CH_2O	30.0		−92.0	−21.00	5.72		(4.90 exp.)		
Ethanal (acetaldehyde)	C_2H_4O	44.1	0.78	−123.0	20.8	5.08		(2.52 exp.)	0.45	
Propanal	C_3H_6O	58.1	0.87	−80.0	48.0	4.63		(2.50 exp.)	0.59	
n-Butanal (butyraldehyde)	C_4H_8O	72.1	0.80	-96.4	74.8	4.19	0.01	2.20 (2.33 exp.)	0.88	
iso-Butanal (isobutyraldehyde)	C_4H_8O	72.1		−65.0	64.1	4.36		(2.10 exp.)		
n-Pentanal (valeraldehyde)	$C_5H_{10}O$	86.1	0.81	−93.5	103.0	3.66		(2.22 exp.)		
Hexanal	$C_6H_{12}O$	100.2	0.85	−56.0	131.0	3.17	1.30	1.92 (2.06 exp.)	1.78	
2-Propenal (acrolein)	C_3H_4O	56.1	0.84	−87.3	52.6	4.56		(2.27 exp.)	−0.01	
Benzaldehyde	C_7H_6O	106.1	1.04	−26.0	178.8	2.24	1.55	2.60 (2.95 exp.)	1.48	
				Ketones						
Propanone (acetone)	C_3H_6O	58.1	0.79	−94.7	56.1	4.50	miscible	(2.80 exp.)	−0.24	
Butanone	C_4H_8O	72.1	0.81	−87.0	79.6	4.09		(2.60 exp.)	0.29	
2-Pentanone	$C_5H_{10}O$	86.1	0.81	−76.9	102.3	3.70	0.16	2.53 (2.58 exp.)	0.90	
2-Hexanone	$C_6H_{12}O$	100.2	0.81	−55.8	128.6	3.20	0.76	2.43	1.38	
Cyclohexanone	$C_6H_{10}O$	98.1	0.95	−32.1	155.6	2.78	0.63	2.98	0.71	
Methyl-phenyl-ketone (acetophenone)	C_8H_8O	120.2	1.03	19.6	202.0	1.67	1.35	3.37	1.63	
Diphenylketone (benzophenone)	$C_{13}H_{10}O$	182.2		48.0	305.4	−1.05	2.82	4.62	3.18	

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–log K_{iaw} calculated (experimental)	log K_{iow}	pK_{ia}
				Carboxylic Acids						
Acetic acid	$C_2H_4O_2$	60.1		16.7	117.9	3.32	miscible	(4.95 exp.)	–0.25	4.75
Propanoic acid	$C_3H_6O_2$	74.1	0.99	–20.7	141.1	2.70	miscible	(4.74 exp.)	0.33	4.87
Butanoic acid (butyric acid)	$C_4H_8O_2$	88.1	0.96	–5.7	163.7	2.18	0.19	4.02 (4.66 exp.)	0.79	4.85
Hexanoic acid	$C_6H_{12}O_2$	116.1	0.93	–3.5	205.0	0.70		(4.56 exp.)	1.92	4.87
Benzoic acid	$C_7H_6O_2$	122.1	1.27	122.4	249.2	–0.96	1.55	5.80	1.89	4.19
Phenylacetic acid	$C_8H_8O_2$	136.2		77.0	265.0	–0.08	0.92	5.55	1.41	4.31
Salicylic acid (2-hydroxy benzoic acid)	$C_7H_6O_3$	138.1	1.44	159.0	211.0	–1.70	1.78	5.31	2.24	2.97 13.40
o-Phthalic acid	$C_8H_6O_4$	166.1		210.0			1.38		0.73	2.89 5.51
				Carboxylic Acid Esters						
Methyl acetate	$C_3H_6O_2$	74.1	0.93	–98.1	56.9	4.46	–0.52	2.45 (2.04 exp.)	0.20	
Ethyl acetate	$C_4H_8O_2$	88.1	0.90	–41.5	77.1	4.10	–0.04	2.33 (2.16 exp.)	0.69	
Propyl acetate	$C_5H_{10}O_2$	102.1	0.89	–95.0	101.5	3.65	0.67	2.07 (2.05 exp.)	1.24	
Butyl acetate	$C_6H_{12}O_2$	116.2	0.88	–73.5	126.1	3.20	1.28	1.91 (1.94 exp.)	1.80	
Hexyl acetate	$C_8H_{16}O_2$	144.2	0.88	–80.9	171.5	2.27	2.46	1.66	2.83	
Vinyl acetate	$C_4H_6O_2$	86.1	0.93	–92.8	72.5	4.15	0.64	1.60	0.73	
Methyl benzoate	$C_8H_8O_2$	136.2	1.09	–12.1	199.5	1.72	1.81	2.86	2.20	
Ethyl benzoate	$C_9H_{10}O_2$	150.2	1.05	–34.0	212.4	1.38	2.63	2.38	2.64	
				Phthalates						
Dimethylphthalate	$C_{10}H_{10}O_4$	194.2	1.19	5.5	283.7	0.38	1.66	4.35	1.53	
Diethylphthalate	$C_{12}H_{14}O_4$	222.2	1.23	–40.5	296.0	–0.66	2.44	4.61	2.39	
Di–*n*-propyl-phthalate	$C_{14}H_{18}O_4$	250.3			304.5		3.36		3.27	
Di-*n*-butyl-phthalate	$C_{16}H_{22}O_4$	278.3	1.05	–35.0	340.0	–2.28	4.36	4.31	4.61	
Benzyl-*n*-butyl-phthalate	$C_{19}H_{20}O_4$	312.4	1.12	<-35.0	370.0	–2.94	5.08	4.25	4.91	
Di-(2-ethylhexyl)-phthalate	$C_{24}H_{38}O_4$	390.6	0.98	–50.0	385.0	–2.72	7.13	1.98	7.48	
				Aromatic Amines						
Aminobenzene (aniline)	C_6H_7N	93.1	1.01	–6.3	184.4	1.92	0.44	4.03	0.95	4.63
2-Methylaniline (*o*-toluidine)	C_7H_9N	107.2	1.00	–16.3	200.3	1.55	0.82	4.02	1.32	4.44

3-Methylaniline (*m*-toluidine)	C_7H_9N	107.2	0.99	–31.5	203.3	1.42	0.85	4.12	1.40	4.72
4-Methylaniline (*p*-toluidine)	C_7H_9N	107.2	1.04	43.7	200.4	1.60	1.15	3.64	1.39	5.17
2,6-Dimethylaniline	$C_8H_{11}N$	121.2	0.98	11.2	214.0	1.30	1.41	3.68	1.84	3.95
3,4-Dimethylaniline	$C_8H_{11}N$	121.2		51.0	228.0		1.65		1.84	5.28
N,N-Dimethylaniline	$C_8H_{11}N$	121.2		2.5	194.0	1.95	2.04	2.40	2.31	5.12
2-Chloroaniline	C_6H_6ClN	127.6	1.21	–14.0	208.8	1.54	1.53	3.32	1.88	2.65
3-Chloroaniline	C_6H_6ClN	127.6	1.22	–10.3	229.5	0.98	1.37	4.04	1.99	3.52
4-Chloroaniline	C_6H_6ClN	127.6	1.43	71.0	231.3	0.40	1.64	4.35	1.83	4.00
3,4-Dichloroaniline	$C_6H_5Cl_2N$	162.0		71.0	272.0	0.36	3.24	2.79	2.70	2.97
N-Phenylaniline (diphenylamine)	$C_{12}H_{11}N$	169.2	1.16	53.0	302.0	–1.22	3.53	4.08	3.50	0.90
4,4'-Diaminobiphenyl (benzidine)	$C_{12}H_{12}N_2$	184.2		120.0	401.0		2.66		1.34	3.57 4.66
1-Naphthylamine	$C_{10}H_9N$	143.2	1.13	49.5	300.9		1.92	5.34	2.25	3.92
2-Naphthylamine	$C_{10}H_9N$	143.2	1.06	111.5	306.0			5.48	2.30	4.15
				Aliphatic Amines						
Methylamine	CH_5N	31.1		–92.5	–6.5	5.55		(3.34 exp.)	–0.57	
Dimethylamine	C_2H_7N	45.1		–96.0	7.4	5.31		(3.15 exp.)	–0.38	10.80
Trimethylamine	C_3H_9N	59.1		–117.2	2.9	5.34		(2.56 exp.)	0.27	9.80
Ethylamine	C_2H_7N	45.1		–81.0	16.6	5.15		(3.30 exp.)	–0.13	10.80
Diethylamine	$C_4H_{11}N$	73.1	0.71	–49.5	56.1	4.50		(2.98 exp.)	0.50	10.90
n-Propylamine	C_3H_9N	59.1	0.72	–83.0	48.7	4.62		(3.22 exp.)	0.32	10.70
n-Buthylamine	$C_4H_{11}N$	73.1	0.74	–50.0	77.9	4.11		(3.11 exp.)	0.98	10.70
n-Hexylamine	$C_6H_{15}N$	101.2	0.77	–22.9	132.8	3.07	0.25	3.07 (2.90 exp.)	2.06	
				Heterocyclic N-Compounds						
Pyridine	C_5H_5N	79.1	0.98	–41.6	115.3	3.44		(3.44 exp.)	0.65	5.25
2-Methylpyridine (2-picoline)	C_6H_7N	93.1	0.94	–66.7	129.4	3.18		(3.40 exp.)	1.11	5.97
3-Methylpyridine (3-picoline)	C_6H_7N	93.1	0.95	–18.1	144.1	3.12		(3.50 exp.)	1.22	5.67
4-Methylpyridine (4-picoline)	C_6H_7N	93.1	0.95	3.7	145.4	2.88		(3.62 exp.)	1.22	5.99
2,3-Dimethylpyridine (2,3-lutidine)	C_7H_9N	107.2	0.94	–15.5	163.5	2.62		(3.54 exp.)	1.65	6.57
2,6-Dimethylpyridine (2,6-lutidine)	C_7H_9N	107.2	0.92	–6.1	144.1	2.87		(3.37 exp.)	1.68	6.65
Quinoline	C_9H_7N	129.2	1.10	–14.8	237.1	0.08	1.33	4.98 (4.20 exp.)	2.06	4.90
Isoquinoline	C_9H_7N	129.2	1.10	26.5	243.2					5.40
				Nitrobenzenes						
Nitrobenzene	$C_6H_5NO_2$	123.1	1.20	5.7	210.8	1.48	1.79	3.12	1.85	
2-Methylnitrobenzene (2-nitrotoluene)	$C_7H_7NO_2$	137.1	1.16	–9.9	222.0	1.43	2.35	2.61	2.30	

Compound Name	Molecular Formula	M_i (g·mol^{-1})	ρ_i (g·cm^{-3})	T_m (°C)	T_b (°C)	log p_i^*/Pa	–log C_{iw}^{sat}	–log K_{iaw} calculated (experimental)	log K_{iow}	pK_{ia}
3-Methylnitrobenzene (3-nitrotoluene)	$C_7H_7NO_2$	137.1		15.9	232.0	1.28	2.43	2.68	2.43	
4-Methylnitrobenzene (4-nitrotoluene)	$C_7H_7NO_2$	137.1	1.39	51.6	238.3	1.20	2.43	2.76	2.38	
2-Chloronitrobenzene	$C_6H_4ClNO_2$	157.6		33.0	245.3	0.70	2.69	3.00 (2.74 exp.)	2.45	
3-Chloronitrobenzene	$C_6H_4ClNO_2$	157.6		45.0	235.6	0.27	2.73	3.39	2.48	
4-Chloronitrobenzene	$C_6H_4ClNO_2$	157.6		83.3	240.5	0.44	2.92	3.03 (2.66 exp.)	2.50	
1,3-Dinitrobenzene	$C_6H_4N_2O_4$	168.1		89.9	301.9	–1.92	2.54	5.77	1.49	
1-Methyl-2,4-dinitrobenzene (2.4-dinitrotoluene)	$C_7H_6N_2O_4$	182.1	1.52	70.3		–1.54	2.86	5.25 (4.80 exp.)	2.00	
1,3-Dinitro-2-methylbenzene (2,6-dinitrotoluene)	$C_7H_6N_2O_4$	182.1	1.28	65.5		–1.12	3.00	4.51	2.03	
1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	213.1		122.9		–1.82	2.81	5.40	1.18	
2-Methyl-1,3,5-trinitrobenzene (2,4,6-trinitrotoluene "TNT")	$C_7H_5N_3O_6$	227.1		80.8		–3.07	3.24	6.22 (5.98 exp.)	1.98	
Triazine-, Carbamide-, Carbamate-, and Urea Pesticides										
Simazine	$C_7H_{12}ClN_5$	201.7	1.30	226.0		–5.07	4.55	6.91	2.18	
Atrazine	$C_8H_{10}ClN_5$	215.7	1.19	175.0		–4.40	3.86	6.93	2.65	
Cyanazine	$C_9H_{13}ClN_6$	240.7		167.0		–6.67	3.15	9.90	2.22	
Propachlor	$C_{11}H_{14}ClNO$	211.7	1.13	71.0		–1.70	2.55	5.54	2.20	
Alachlor	$C_{14}H_{20}ClNO$	269.8	1.13	41.0		–2.70	3.05	6.04	2.95	
Metolachlor	$C_{15}H_{22}ClNO_2$	283.8		<25		–2.40	2.75	6.04	3.13	
Carbaryl	$C_{12}H_{11}NO_2$	201.2	1.23	142.0		–4.57	3.22	7.74	2.36	
Carbofuran	$C_{12}H_{15}NO_3$	221.3	1.18	152.5		–4.12	2.81	7.70	1.52	
Fenuron	$C_9H_{12}N_2O$	164.2	1.08	135.5			1.63		0.98	
Diuron	$C_9H_{10}Cl_2N_2O$	233.1	1.48	158.5		<–4.0	3.76		2.60	
Isoproturon	$C_{12}H_{18}N_2O$	206.3	1.16	155.5		<–4.0	3.57		2.50	
Phosphoric- and Thiophosphoric Acid (Thio)Esters										
Tributylphosphate	$C_{12}H_{27}O_4P$	263.3	0.98	<0		–0.10	2.65	3.84	2.50	
Tri-*o*-cresylphosphat	$C_{21}H_{21}O_4P$	368.4	1.21	50		–3.00	5.31	4.08	5.11	
Parathion	$C_{10}H_{14}NO_5PS$	291.3	1.27	6.1		–3.22	4.30	5.31	3.81	
Methylparathion	$C_8H_{10}NO_5PS$	263.5	1.36	37.5		–2.70	4.00	5.10	3.00	
Fenthion	$C_{10}H_{15}O_3PS_2$	278.3	1.25	7.5		–2.70	3.74	5.35	4.10	
Disulfoton	$C_8H_{19}O_2PS_3$	274.4	1.14	<25		–1.80	4.20	4.00	4.02	