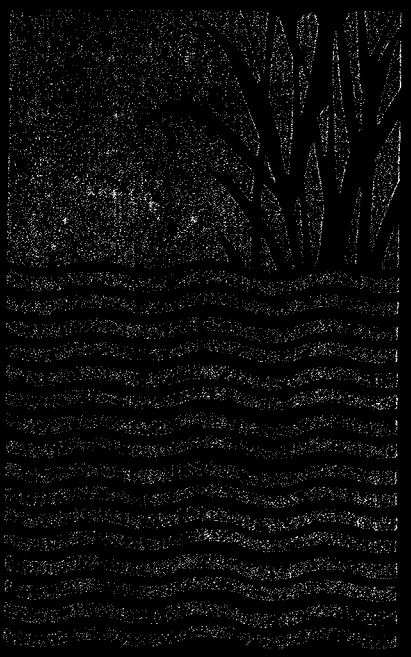
ENVIRONMENTAL ORGANIC CHEMISTRY



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ENVIRONMENTAL ORGANIC CHEMISTRY

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APPENDIX

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm) $-\log P^0$	Vapor Pressure at 25°C (atm) $-\log P^0$(L) (For Solids and Gases)	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$(L) (For Solids and Gases)	Henry's Law Constant at 25°C (L atm mol^{-1}) $\log K_H$ Calculated	Henry's Law Constant at 25°C (L atm mol^{-1}) $\log K_H$ (Experimental)	Octanol–Water Partition Coefficient at 25°C [(mol·L^{-1} octanol)·(mol·L^{-1} water)$^{-1}$] $\log K_{ow}$
Saturated and Unsaturated Hydrocarbons											
Methane	CH_4	16.0	−182.5	−164.0		−2.44	2.82[a]	0.38[a]		2.82	1.09
Ethane	C_2H_6	30.1	−183.3	−88.6		−1.60	2.69[a]	1.09[a]		2.69	1.81
Propane	C_3H_8	44.1	−189.7	−42.1		−0.97	2.85[a]	1.88[a]		2.85	2.36
n-Butane	C_4H_{10}	58.1	−138.4	−0.5		−0.39	2.98[a]	2.59[a]		2.98	2.89
n-Pentane	C_5H_{12}	72.2	−129.7	36.1	0.16		3.25			3.09	3.62
n-Hexane	C_6H_{14}	86.2	−95.0	69.0	0.69		3.83			3.14	4.11
n-Heptane	C_7H_{16}	100.2	−90.6	98.4	1.21		4.51			3.30	4.66
n-Octane	C_8H_{18}	114.2	−56.8	125.7	1.73		5.20			3.47	5.18
n-Nonane	C_9H_{20}	128.3	−51.0	150.8	2.24		5.94			3.70	
n-Decane	$C_{10}H_{22}$	142.3	−29.7	174.1	2.76		6.57			3.81	
n-Dodecane	$C_{12}H_{26}$	170.3	−9.6	216.3	3.80		7.52			3.72	
n-Hexadecane	$C_{16}H_{34}$	226.4	18.2	287.0	5.73		7.80			2.07	
n-Octadecane	$C_{18}H_{38}$	254.4	28.2	316.1	6.67		8.08			1.41	
Cyclohexane	C_6H_{12}	84.2	6.6	80.7	0.90		3.15			2.25	3.44
1-Hexene	C_6H_{12}	84.2	−139.8	63.4	0.60		3.15			2.45	3.39
1-Octene	C_8H_{16}	112.2	−101.7	121.3	1.63		4.52			2.89	4.57
Miscellaneous Aliphatic Compounds[c]											
1-Butanol	$C_4H_{10}O$	74.1	−89.5	117.2	2.02		0.07		−1.95		0.79
1-Hexanol	$C_6H_{14}O$	102.2	−46.7	158.0	2.85		0.88				2.03
1-Octanol	$C_8H_{18}O$	130.2	−16.7	194.4			2.35				2.84
1-Nonanol	$C_9H_{20}O$	144.2	−5.5	213.5	4.00		3.13				3.77
2-Ethyl-1,3-hexanediol	$C_8H_{18}O_2$	146.2	−40.0	244.0			2.81				3.22
Cyclohexanol	$C_6H_{12}O$	100.2	25.1	161.1	2.70	2.70	0.42	0.42	−2.28		1.23
Acetone	C_3H_6O	58.1	−94.6	56.5	0.55		−1.13		−1.68		−0.24
									−1.44		

2-Octanone	$C_8H_{16}O$	128.2	−16.0	172.9	2.88		2.05		−0.83	2.76
2-Decanone	$C_{10}H_{20}O$	156.2	3.5	211.0	3.45		3.30		−0.15	3.81
n-Butylacetate	$C_6H_{12}O_2$	116.2	−77.9	126.5						1.78
1-Bromohexane	$C_6H_{13}Br$	165.1	−84.7	155.3						4.65
1-Bromoheptane	$C_7H_{15}Br$	179.1	−56.1	178.5						5.23
1-Bromooctane	$C_8H_{17}Br$	193.1	−55.0	200.8			5.06			5.82
				Substituted Benzenes[d]						
Benzene	C_6H_6	78.1	5.5	80.1	0.90		1.64		0.74 (0.75 exp.)	2.13
Toluene	C_7H_8	92.1	−95.0	110.6	1.42		2.25		0.83 (0.83 exp.)	2.69
Ethylbenzene	C_8H_{10}	106.2	−95.0	136.2	1.90		2.80		0.90 (0.93 exp.)	3.15
1,2-Dimethyl-benzene	C_8H_{10}	106.2	−25.2	144.4	2.05		2.76		0.71	3.12
1,4-Dimethyl-benzene	C_8H_{10}	106.2	13.2	138.0	1.93		2.77		0.84	3.18
n-Propylbenzene	C_9H_{12}	120.2	−101.6	159.2	2.35		3.34		0.99	3.63
1,2,4-Tri-methylbenzene	C_9H_{12}	120.2	−43.8	169.4	2.57		3.33		0.76	3.65
1,3,5-Tri-methylbenzene	C_9H_{12}	120.2	−44.7	164.7	2.48		3.40		0.92	3.42
n-Butylbenzene	$C_{10}H_{14}$	134.2	−88.0	183.0	2.86		3.97		1.13	4.28
n-Pentylbenzene	$C_{11}H_{16}$	148.3	−75.0	205.4	3.36		4.59		1.23	4.90
Chlorobenzene	C_6H_5Cl	112.6	−45.6	132.0	1.80		2.35		0.55 (0.54 exp.)	2.92
1,2-Dichloro-benzene	$C_6H_4Cl_2$	147.0	−17.0	180.0	2.71		3.20, 3.01		0.49, 0.29 (0.28 exp.)	3.38
1,4-Dichloro-benzene	$C_6H_4Cl_2$	147.0	53.1	174.0	3.04	2.76	3.39	3.11	0.35	3.38
1,2,4-Trichloro-benzene	$C_6H_3Cl_3$	181.5	16.9	213.5	3.21		3.65		0.44	4.00
1.3,5-Trichloro-benzene	$C_6H_3Cl_3$	181.5	63.0	208.0	3.49	3.11	4.53	4.15	1.04	4.02

Appendix (*Continued*)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm) $-\log P^0$	Vapor Pressure at 25°C (atm) $-\log P^0$(L) (For Solids and Gases)	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$(L) (For Solids and Gases)	Henry's Law Constant at 25°C (L atm mol^{-1}) $\log K_H$ Calculated (Experimental)	Octanol–Water Partition Coefficient at 25°C [(mol·L^{-1} octanol)·(mol·L^{-1} water)$^{-1}$] $\log K_{ow}$
1,2,3,4-Tetrachlorobenzene	$C_6H_2Cl_4$	215.9	47.5	254.0	4.28	4.06	4.42	4.20	0.14	4.55
1,2,3,5-Tetrachlorobenzene	$C_6H_2Cl_4$	215.9	54.5	246.0	4.01	3.73	4.83	4.55	0.82	4.65
Pentachlorobenzene	C_6HCl_5	250.3	86.0	277.0	4.66	4.05	5.56	4.95	0.90	5.03
Hexachlorobenzene	C_6Cl_6	284.8	230.0	322.0	7.51	5.46	7.69	5.64	0.18	5.50
Bromobenzene	C_6H_5Br	157.0	−30.8	156.0	2.25		2.64		0.41 (0.39 exp.)	2.99
1,4-Dibromobenzene	$C_6H_4Br_2$	235.9	87.3	219.0	3.67	3.05	4.07	3.45	0.40	3.75
4-Bromochlorobenzene	C_6H_4BrCl	191.5	68.0	196.0	3.46	3.03	3.63	3.20	0.17	3.53
Fluorobenzene	C_6H_5F	96.1	−41.2	85.1	1.00		1.79		0.79	2.27
Phenol	C_6H_6O	94.1	43.0	181.7	3.59	3.41	0.20	0.02	−3.39	1.45
3-Methyl phenol (*m*-cresol)	C_7H_8O	108.6	11.5	202.2			1.59			1.96
2,4-Dimethyl phenol	$C_8H_{12}O$	122.2	27.5	210.0			1.19	1.17		2.35
2-Chlorophenol	C_6H_5ClO	128.6	9.0	174.9			1.05			2.16
Aniline	C_6H_7N	93.1	−6.3	184.0	2.89		0.41		−2.48	0.90
N-Methylaniline	C_7H_9N	107.2	−57.0	196.3			1.28			1.66
N-Dimethyl-										

Aniline	C_6H_7N	93.1	−6.3	184.4			1.28			1.66
N-Methyl-aniline	C_7H_9N	107.2	−57.0	196.3						
N-Dimethyl-aniline	$C_8H_{11}N$	121.2	2.5	194.0			2.04			2.31
Nitrobenzene	$C_6H_5NO_2$	123.1	5.7	210.8			1.77			1.83
Benzaldehyde	C_7H_6O	106.1	−26.0	178.0	2.90		1.51		−1.39	1.48
Polycyclic Aromatic Hydrocarbons[e]										
Naphthalene	$C_{10}H_8$	128.2	80.6	217.9	3.98	3.43	3.61	3.06	−0.37 (−0.31 exp.)	3.36
Fluorene	$C_{13}H_{10}$	166.2	113.0	295.0	6.10	5.22	4.96	4.08	−1.14 (−1.00 exp.)	4.18
Phenanthrene	$C_{14}H_{10}$	178.2	99.5	340.2	6.79	6.05	5.20	4.46	−1.59 (−1.45 exp.)	4.57
Anthracene	$C_{14}H_{10}$	178.2	217.5	342.0	8.10	6.11	6.46	4.48	−1.64	4.54
Fluoranthrene	$C_{16}H_{10}$	202.3	110.8		7.91	7.06	5.93	5.08	−1.98	5.22
Pyrene	$C_{16}H_{10}$	202.3	156.0		8.22	7.40	6.17	5.35	−2.05 (−1.96 exp.)	5.13
Benz(a)anthracene	$C_{18}H_{12}$	228.3	159.8	435.0	9.55	8.20	7.31	5.96	−2.24	5.91
Benzo(a)pyrene	$C_{20}H_{12}$	252.3	176.5		11.14	9.63	8.22	6.71	−2.92	6.50
Phthalates[f]										
Dimethyl phthalate	$C_{10}H_{10}O_4$	194.2	<25	283.7	4.62		1.66		−2.96	1.53
Diethyl phthalate	$C_{12}H_{14}O_4$	222.2	<25	298.0	5.08		2.38		−2.70	2.35
Di-*n*-propyl phthalate	$C_{14}H_{18}O_4$	250.3	<25	304.5			3.36			3.27
Diisobutyl phthalate	$C_{16}H_{22}O_4$	278.3	<25	296.5			4.13			4.11
Di-*n*-butyl phthalate	$C_{16}H_{22}O_4$	278.3	<25	340.0	7.02		4.47		−2.89	4.57

Appendix (*Continued*)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm) $-\log P^0$	Vapor Pressure at 25°C (atm) $-\log P^0$(L) (For Solids and Gases)	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$(L) (For Solids and Gases)	Henry's Law Constant at 25°C (L atm mol^{-1}) $\log K_H$ Calculated (Experimental)	Octanol–Water Partition Coefficient at 25°C [(mol·L^{-1} octanol)·(mol·L^{-1} water)$^{-1}$] $\log K_{ow}$
					Halogenated C_1–C_4 Compounds[a]					
Chloromethane	CH_3Cl	50.5	−97.7	−24.2		−0.76	0.98[a]	0.22	0.98	0.91
Dichloromethane	CH_2Cl_2	84.9	−95.1	39.7	0.23		0.64		0.41 (0.43 exp.)	1.15
Trichloromethane	$CHCl_3$	119.4	−63.5	61.7	0.59		1.19		0.60 (0.59 exp.)	1.93
Tetrachloromethane	CCl_4	153.8	−22.9	76.5	0.82		2.20		1.38 (1.33 exp.)	2.73
1,1-Dichloroethane	$C_2H_4Cl_2$	99.0	−97.0	57.5	0.52		1.30		0.78	1.79
1,2-Dichloroethane	$C_2H_4Cl_2$	99.0	−35.4	83.5	1.04		1.07		0.03 (0.00 exp.)	1.47
1,1,1-Trichloroethane	$C_2H_3Cl_3$	133.4	−30.4	74.1	0.78		2.07		1.29	2.48
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	167.9	−36.0	146.2	2.06		1.74		−0.32	2.39
Chloroethene (vinyl chloride)	C_2H_3Cl	62.5	−153.8	−13.4		−0.59	1.35[a]	0.76	1.35	0.60
Trichloroethene	C_2HCl_3	131.4	−73.0	87.0	1.01		2.04		1.03	2.42
Tetrachloroethene	C_2Cl_4	165.8	−19.0	121.0	1.60		3.04		1.44	2.88

ethene	C_2Cl_4	165.8	−19.0	121.0	1.60		3.04		1.44	2.88
Hexachloro-butadiene	C_4Cl_6	260.8	−21.0	215.0	3.46 (calc)		4.90		1.44	4.90
Bromomethane	CH_3Br	94.9	−93.6	3.6		−0.26	0.79[a]	0.53	0.79	1.19
Tribromo-methane	$CHBr_3$	252.8	8.3	149.5	2.13		1.91		−0.22	
1,2-Dibromo-ethane	$C_2H_4Br_2$	187.9	−34.2	167.3	2.57		2.04		−0.53	
1,2-Dibromo-3-chloro-propane	$C_3H_5Br_2Cl$	236.4		178.0	2.90		2.44		−0.46	
Trichloro-fluoromethane	CCl_3F	137.4	−111.0	23.8		−0.02	2.10[a]	2.08	2.10	2.16
Dichlorodi-fluoromethane	CCl_2F_2	120.9	−158.0	−29.8		−0.80	2.60[a]	1.80	2.60	2.53
					Polychlorinated Biphenyls (PCBs)[b]					
Biphenyl	$C_{12}H_{10}$	154.2	71.0	255.9		5.00		3.88		4.09
2-CBP	$C_{12}H_9Cl$	188.6	32.1		4.66	4.60	4.57	4.51	−0.09	4.53
4-CBP	$C_{12}H_9Cl$	188.6	77.7		5.76	5.23	5.13	4.58	−0.63	4.40
2,5-CBP	$C_{12}H_8Cl_2$	223.1	23.0		5.53		5.06		−0.47	5.22
4,4′-CBP	$C_{12}H_8Cl_2$	223.1	149.0		7.32	6.08	6.53	5.29	−0.79	5.33
2,4,5-CBP	$C_{12}H_7Cl_3$	257.5	76.3		6.95	6.36	6.26	5.67	−0.69	5.74
2′,3,4-CBP	$C_{12}H_7Cl_3$	257.5	60.0		6.88	6.53	6.52	6.17	−0.36	5.78
2,2′,5,5′-CBP	$C_{12}H_6Cl_4$	292.0	87.0		7.60	6.64	7.06	6.10	−0.54	6.18
2,3′,4,4′-CBP	$C_{12}H_6Cl_4$	292.0	128.0		8.21	7.18	7.70	6.67	−0.51	6.31
2,2′,4,5,5′-CBP	$C_{12}H_5Cl_5$	326.4	77.0		8.02	7.40	7.40	6.78	−0.62	6.36
2,2′,4,4′,5,5′-CBP	$C_{12}H_4Cl_6$	360.9	103.0		8.97	8.15	7.82	7.00	−1.15	7.15
2,2′,3,3′,4,4′-CBP	$C_{12}H_4Cl_6$	360.9	151.9		9.65	8.38	8.72	7.45	−0.93	6.97
2,2′,3,3′,4,4′,6-CBP	$C_{12}H_3Cl_7$	395.3	122.3		9.40	8.53	8.26	7.48	−1.14	6.68
2,2′,3,3′,5,5′,6,6′-CBP	$C_{12}H_2Cl_8$	429.8	161.0		9.54	8.29	9.29	8.04	−1.25	7.12
Decachloro-BP	$C_{12}Cl_{10}$	498.7	305.8		12.28	9.85	10.55	8.12	−1.73	8.23

Appendix (*Continued*)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm) $-\log P^0$	Vapor Pressure at 25°C (atm) $-\log P^0$(L) (For Solids and Gases)	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$	Aqueous Solubility at 25°C (mol L^{-1}) $-\log C_w^{sat}$(L) (For Solids and Gases)	Henry's Law Constant at 25°C (L atm mol^{-1}) $\log K_H$ Calculated (Experimental)	Octanol–Water Partition Coefficient at 25°C [(mol·L^{-1} octanol)·(mol·L^{-1} water)$^{-1}$] $\log K_{ow}$
					Sulfur-Containing Compounds[i]					
Dimethyl sulfide	C_2H_6S	62.13	−98.0	37.3	0.20		0.45		(0.25)	
Diethyl sulfide	$C_4H_{10}S$	90.19	−103.8	92.1	1.12		1.34		(0.22)	1.95
Di-*n*-propyl sulfide	$C_6H_{14}S$	118.24	−102.5	142.4	2.10		2.58		(0.48)	
Diisopropyl sulfide	$C_6H_{14}S$	118.24	−78.1	120.0	1.72		2.24		(0.52)	
Dimethyl sulfide	$C_2H_6S_2$	94.20	−84.7	109.7	1.42		1.44		(0.02)	1.77
Diethyl sulfide	$C_4H_{10}S_2$	122.25	−101.5	154.0	2.20		2.42		(0.22)	
Thiophene	C_4H_4S	84.14	−38.2	84.2	0.98		1.33		(0.35)	1.81
2-Methyl thiophene	C_5H_6S	98.17	−63.4	112.6	1.46		1.85		(0.39)	
Methanethiol	CH_4S	48.11	−123.0	6.2		−0.300		0.091	(0.39)	
Ethanethiol	C_2H_6S	62.13	−144.4	35.0	0.16		0.71		(0.55)	
n-Propanethiol	C_3H_8S	76.17	−113.3	67.7	0.69		1.30		(0.61)	
					Miscellaneous Pesticides and Other Compounds[j]					
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin	$C_{12}H_4O_2Cl_4$	322.0	305	421	11.6	8.8	10.3	7.5	−1.3	6.64
Lindane (γ-hexachlorocyclohexane)	$C_6H_6Cl_6$	290.8	112.9		7.08	6.20	4.59	3.71	−2.49	3.78
Dieldrin	$C_{12}H_8Cl_6O$	380.9	175.0		8.18	6.68	6.23	4.98	−1.95	5.48
p,p'-DDT	$C_{14}H_9Cl_5$	354.5	109.0		9.87	9.03	7.85	7.01	−2.02	6.36
Parathion	$C_{10}H_{14}NO_5PS$	291.3	6.1		7.65		4.23		−3.42	3.81
Malathion	$C_{10}H_{19}O_6PS_2$	330.4	2.9				3.36			2.90

Malathion	$C_{10}H_{19}O_6PS_2$	330.4	2.9		3.36		2.89
Phosmit	$C_{11}H_{12}NO_4PS_2$	317.3	72.0	9.22 (20°C)	4.10	3.63	2.83
Dialifos	$C_{14}H_{17}ClNO_4PS_2$	393.9	68.0	10.08 (30°C)	6.34	5.91	4.69
Carbaryl	$C_{12}H_{11}NO_2$	201.2	142.0		3.70	2.53	2.36
Carbofuran	$C_{12}H_{15}NO_3$	221.3	151.0		2.73	1.47	1.60
Fluometuron	$C_{10}H_{11}F_3NO_2$	232.2	164.0		3.51	1.39	1.34
Atrazine	$C_8H_{14}ClN_5$	215.7	174.0		3.81	2.33	2.56
RDX (1,3,5-triaza-1,3,5-trinitrocyclohexane)	$C_3H_6N_6O_6$	222.1	205.0		4.57	2.77	0.87
Tributylphosphate	$C_{12}H_{27}PO_4$	266.3	<25		5.98		4.00
Tri-*o*-cresylphosphate	$C_{21}H_{21}PO_4$	368.4	77.0		6.01	5.49	5.11

[a] At 1 atm.

[b] Hansch and Leo (1979); Mackay and Shiu (1981); Stein (1981); Tewari et al. (1982).

[c] Hansch and Leo (1979); CRC 1985–1986; Tewari et al. (1982).

[d] Hansch and Leo (1979); Yalkowsky and Valvani (1979); Yalkowsky et al. (1979); Banerjee et al. (1980); CRC 1985–1986; Mackay and Shiu (1981); Chiou et al. (1982); Horvath (1982); Tewari et al. (1982); Miller et al. (1984).

[e] Wauchope and Getzen (1972); Mackay et al. (1980a); May et al. (1983); Sonnefeld et al. (1983); Whitehouse (1984).

[f] Wolfe et al. (1980); CRC 1985–1986; Leyder and Boulanger (1983).

[g] Hansch and Leo (1979); Banerjee et al. (1980); Mackay and Shiu (1981); Horvath (1982).

[h] Mackay et al. (1980b); Westcott et al. (1981); Bidleman (1984); Burkhard et al. (1984); Miller et al. (1984); Rapaport and Eisenreich (1984); Woodburn et al. (1984); Burkhard et al. (1985).

[i] Hansch and Leo (1979); CRC 1985–1986; Przyjazny et al. (1983).

[j] Banerjee et al. (1980); Mackay and Shiu (1981); Lyman (1982a,b); Monsanto Company (1985); Marple et al. (1986a,b); Eltzer and Hites (1988).