

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 therein) 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_f (g·mol ⁻¹)	ρ_f (g·cm ⁻³)	T_m (°C)	T_b (°C)	$\log p^*/\text{Pa}$	$-\log C_{f/w}^{\text{sat}}$	$-\log K_{f/w}^{\text{calculated}}$ (experimental)	$\log K_{f/w}$	$pK_{f/a}$
<i>n-Alkanes</i>										
Methane	CH ₄	16.0		-182.5	-164.0	7.45	2.82 (1bar)	-1.43	1.09	
Ethane	C ₂ H ₆	30.1		-183.3	-88.6	6.61	2.69 (1bar)	-1.30	1.81	
Propane	C ₃ H ₈	44.1		-189.7	-42.1	5.98	2.85 (1bar)	-1.46	2.36	
<i>n</i> -Butane	C ₄ H ₁₀	58.1	0.58 (L)	-138.4	-0.5	5.40	2.98 (1bar)	-1.58	2.89	
<i>n</i> -Pentane	C ₅ H ₁₂	72.2	0.63	-129.7	36.1	4.83	3.25	-1.69	3.39	
<i>n</i> -Hexane	C ₆ H ₁₄	86.2	0.66	-95.0	69.0	4.30	3.83	-1.74	4.00	
<i>n</i> -Heptane	C ₇ H ₁₆	100.2	0.68	-90.6	98.4	3.79	4.53	-1.93	4.66	
<i>n</i> -Octane	C ₈ H ₁₈	114.2	0.70	-56.8	125.7	3.26	5.20	-2.07	5.15	
<i>n</i> -Nonane	C ₉ H ₂₀	128.3	0.72	-51.0	150.8	2.76	5.77	-2.14	5.65	
<i>n</i> -Decane	C ₁₀ H ₂₂	142.3	0.73	-29.7	174.1	2.24	6.42	-2.27	6.25	
<i>n</i> -Undecane	C ₁₁ H ₂₄	156.3	0.74	-25.6	195.9	1.72				
<i>n</i> -Dodecane	C ₁₂ H ₂₆	170.3	0.75	-9.6	216.3	1.19	7.52	-2.32		
<i>n</i> -Hexadecane	C ₁₆ H ₃₄	226.4	0.77	18.2	287.0	-0.73	7.80	-0.68		
<i>n</i> -Octadecane	C ₁₈ H ₃₈	254.4	0.78	28.2	316.1	-1.78	8.08	-0.09		
<i>Branched Alkanes</i>										
2-Methylpropane (isobutane)	C ₄ H ₁₀	58.1	0.56 (L)	-159.4	-11.7	5.56	3.07 (1bar)	-1.68	2.82	
2-Methylbutane (isopentane)	C ₅ H ₁₂	72.2	0.62	-159.9	27.9	4.96	3.18	-1.75		
2,2-Dimethylpropane (neopentane)	C ₅ H ₁₂	72.2	0.59 (L)	-16.6	9.5	5.24	3.34 (1bar)	-1.95	3.11	
2-Methylpentane (isohexane)	C ₆ H ₁₄	86.2	0.64	-153.8	60.1	4.45	3.80	-1.86	3.60	
2,2-Dimethylbutane (neohexane)	C ₆ H ₁₄	86.2	0.65	-99.8	49.7	4.63	3.65	-1.89	3.42	
2,2,4-Trimethylpentane (isooctane)	C ₈ H ₁₈	114.2	0.69	-107.4	99.2	3.81	4.67	-2.09		
<i>Unsaturated and Alicyclic Hydrocarbons</i>										
1,3-Butadiene	C ₄ H 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 ₅ H ₈	68.1	0.68	-146.0	34.0	4.86	2.04	-0.51	2.05	
1,4-Pentadiene	C ₅ H ₈	68.1	0.66	-148.3	26.0	5.00	2.08	-0.69		
Cyclopentene	C ₅ H ₈	68.1	0.77	-135.1	44.2	4.70	2.09	-0.40		
Cyclopentane	C ₅ H ₁₀	70.1	0.74	-92.9	49.2	4.63	2.64	-0.88	3.00	
1,4-Cyclohexadiene	C ₆ H ₈	80.1	0.85	-49.2	81.5	3.95	2.03	0.41	2.30	
Cyclohexene	C ₆ H ₁₀	82.1	0.81	-103.5	83.0	4.07	2.60	-0.28	2.86	
Cyclohexane	C ₆ H ₁₂	84.2	0.78	6.5	80.7	4.10	3.17	-0.89	3.44	
1-Hexene	C ₆ H ₁₂	84.2	0.67	-139.8	63.4	4.40	3.22	-1.22	3.40	
Methylcyclohexane	C ₇ H ₁₄	98.2	0.77	-126.6	100.6	3.79	3.81	-1.21	3.88	

Alkylated Benzenes

Benzene	C ₆ H ₆	78.1	0.88	5.5	80.1	4.10	1.65	0.65 (0.65 exp.)	2.17
Methylbenzene (toluene)	C ₇ H ₈	92.2	0.87	-95.0	110.6	3.57	2.22	0.60 (0.62 exp.)	2.69
Ethylbenzene	C ₈ H ₁₀	106.2	0.86	-95.0	136.2	3.09	2.80	0.50 (0.47 exp.)	3.20
Vinylbenzene (styrene)	C ₈ H ₈	104.2	0.91	-31.0	145.1	2.94	2.53	0.93 (0.92 exp.)	2.95
1,2-Dimethylbenzene (<i>o</i> -xylene)	C ₈ H ₁₀	106.2	0.88	-25.2	144.4	2.95	2.75	0.69 (0.68 exp.)	3.16
1,3-Dimethylbenzene (<i>m</i> -xylene)	C ₈ H ₁₀	106.2	0.86	-47.8	139.1	3.04	2.82	0.53 (0.52 exp.)	3.30
1,4-Dimethylbenzene (<i>p</i> -xylene)	C ₈ H ₁₀	106.2	0.86	13.3	138.1	3.07	2.77	0.55 (0.54 exp.)	3.27
<i>n</i> -Propylbenzene	C ₉ H ₁₂	120.2	0.86	-99.6	159.2	2.65	3.34	0.40	3.69
Isopropylbenzene	C ₉ H ₁₂	120.2	0.86	-96.6	154.2	2.79	3.33	0.27	3.66
1,2,3-Trimethylbenzene	C ₉ H ₁₂	120.2	0.89	-25.4	176.1	2.30	3.23	0.86	3.60
1,2,4-Trimethylbenzene	C ₉ H ₁₂	120.2	0.88	-43.8	169.4	2.42	3.33	0.65	3.65
1,3,5-Trimethylbenzene	C ₉ H ₁₂	120.2	0.88	-44.7	164.7	2.52	3.38	0.50	3.42
1-Ethyl-2-methylbenzene	C ₉ H ₁₂	120.2	0.88	-83.8	165.2	2.52	3.20	0.67	3.53
1-Ethyl-4-methylbenzene	C ₉ H ₁₂	120.2	0.86	-62.4	162.0	2.60	3.10	0.69	3.63
<i>n</i> -Butylbenzene	C ₁₀ H ₁₄	134.2	0.86	-88.0	183.0	2.15	3.95	0.29	4.38
<i>s</i> -Butylbenzene	C ₁₀ H ₁₄	134.2	0.86	-75.0	174.0	2.40	3.73	0.26	4.44
<i>t</i> -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
<i>n</i> -Pentylbenzene	C ₁₁ H ₁₆	148.3	0.86	-78.3	202.2	1.65	4.59	0.15	4.90
<i>n</i> -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 ₉ H 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)	$\log p_i^*/\text{Pa}$	$-\log C_{i,w}^{\text{sat}}$	$-\log K_{i,w}$ calculated (experimental)	$\log K_{i,w}$	$pK_{i,a}$
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	
<i>Chlorinated C₁- to C₄-Compounds</i>										
Chloromethane	CH ₃ Cl	50.5	0.92 (L)	-97.7	-24.2	5.76	0.98 (1bar)	0.42	0.91	
Dichloromethane	CH ₂ Cl 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 ₂ H ₄ Cl ₂	99.0	1.18	-97.3	57.3	4.49	1.29	0.61 (0.62 exp.)	1.79	
1,2-Dichloroethane	C ₂ H ₄ Cl 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 ₂ H ₃ Cl 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 ₂ H ₃ Cl 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 ₂ H ₂ Cl ₄	167.9	1.60	-40.8	146.3	2.90	1.71	1.78 (1.85 exp.)	2.39	
Pentachloroethane	C ₂ HCl ₅	202.3	1.68	-29.0	160.8	2.79	2.61	0.99	3.22	
Hexachloroethane	C ₂ Cl ₆	236.7	2.09	187.5	187.5	1.70	3.68	1.01	3.93	
Chloroethene	C ₂ H ₃ Cl	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 ₂ H ₂ Cl ₂	96.9	1.22	-122.0	31.7	4.90	1.59	-0.10 (-0.03 exp.)	1.48	
<i>cis</i> -1,2-Dichloroethene	C ₂ H ₂ Cl ₂	96.9	1.27	-81.0	60.0	4.45	1.28	0.66 (0.79 exp.)	1.86	
<i>trans</i> -1,2-Dichloroethene	C ₂ H ₂ Cl ₂	96.9	1.27	-50.0	48.0	4.61	1.19	0.59 (0.46 exp.)	2.09	

Trichloroethene	C ₂ HCl ₃	131.4	1.46	-73.0	87.0	4.00	2.08	0.31 (0.40 exp.)	2.42
Tetrachloroethene	C ₂ Cl 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 ₃ H ₅ Cl	76.5	0.94	-135.0	44.9	4.70	1.33	0.36 (0.42 exp.)	1.45
<i>Brominated and Iodated C₁- and C₂-Compounds</i>									
Bromomethane	CH ₃ Br	94.9	1.68 (L)	-93.6	3.6	5.34	0.79 (1bar)	0.35	1.19
Dibromomethane	CH ₂ Br 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 ₂ H ₅ Br	109.0	1.45	-119.0	38.4	4.80	1.09	1.50	1.61
1,2-Dibromoethane	C ₂ H ₄ Br ₂	187.9	2.18	9.8	131.5	3.21	1.63	1.55	1.96
Bromoethene	C ₂ H ₃ Br	107.0	1.49 (L)	-139.5	15.8	5.15	1.01	0.66	1.57
Iodomethane	CH ₃ I	141.9	2.28	-66.5	42.5	4.73	1.01	(0.65 exp.)	1.51
Iodoethane	C ₂ H ₅ I	156.0	1.94	-111.0	72.4	4.26	1.60	0.53	2.00
<i>Mixed Halogenated C₁- and C₂-Compounds</i>									
Bromochloromethane	CH ₂ BrCl	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 ₂ F 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 ₃ F	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 ₂ Cl ₃ F 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 ₂ Cl ₄ F ₂	203.8	1.64	-25.5	92.8	3.87	3.23	-0.71	3.73
<i>Chlorobenzenes</i>									
Chlorobenzene	C ₆ H ₅ Cl	112.6	1.11	-45.2	132.0	3.20	2.39	0.80 (0.82 exp.)	2.78
1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.0	1.30	-17.0	180.0	2.30	3.05	1.04 (1.00 exp.)	3.40
1,3-Dichlorobenzene	C ₆ H ₄ Cl ₂	147.0	1.29	-24.7	173.0	2.45	3.08	0.86 (0.82 exp.)	3.47
1,4-Dichlorobenzene	C ₆ H ₄ Cl 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 ₆ H ₃ Cl ₃	181.5	1.69	52.0	218.5	1.45	3.94	1.01	4.14
1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃	181.5	1.45	17.0	213.5	1.58	3.78	1.03	4.06
1,3,5-Trichlorobenzene	C ₆ H ₃ Cl ₃	181.5	1.39	63.5	208.0	1.50	4.53	0.36	4.19

Compound Name	Molecular Formula	M_f (g mol ⁻¹)	ρ_f (g cm ⁻³)	T_m (°C)	T_b (°C)	log p^*/Pa	$-\log C_{f/w}^{sat}$	$-\log K_{f/w}^{calculated}$ (experimental)	log $K_{f/w}$	p $K_{f/a}$
1,2,3,4-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.9		47.5	254.0	0.75	4.69	0.95	4.64	
1,2,3,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.9	1.86	54.5	246.0	1.00	4.79	0.60	4.66	
1,2,4,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.9		140.0	243.0	-0.14	5.23	1.30	4.72	
Pentachlorobenzene	C ₆ HCl ₅	250.3	1.83	86.0	277.0	-0.66	5.58	1.47	5.18	
Hexachlorobenzene	C ₆ Cl ₆	284.8	2.08	230.0	322.0	-2.60	7.55	1.44 (1.54 exp.)	5.80	
<i>Polychlorinated Biphenyls (PCBs), Selected Congeners</i>										
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 ₉ Cl	188.6	0.98	34.0	274.0	-0.30	4.54	1.55	4.53	
4-CBP (PCB3)	C ₁₂ H ₉ Cl	188.6	0.98	77.7	291.0	-0.57	5.19	1.77	4.61	
2,2'-CBP (PCB4)	C ₁₂ H ₈ Cl ₂	223.1	1.05	61.0		-0.58	5.35	1.62	4.97	
2,4-CBP (PCB7)	C ₁₂ H ₈ Cl ₂	223.1	1.05	24.4		-0.60	5.25	1.74	5.30	
2,4'-CBP (PCB8)	C ₁₂ H ₈ Cl ₂	223.1	1.05	45.0		-1.10	5.35	2.14	5.10	
4,4'-CBP (PCB15)	C ₁₂ H ₈ Cl ₂	223.1	1.05	148.5		-2.30	6.57	2.12	5.33	
2,2',5-CBP (PCB18)	C ₁₂ H ₇ Cl ₃	257.5	1.15	44.0		-0.84	5.80	1.43	5.60	
2,4,4'-CBP (PCB28)	C ₁₂ H ₇ Cl ₃	257.5	1.15	57.5		-1.70	6.20	1.89	5.62	
2,4,5-CBP (PCB29)	C ₁₂ H ₇ Cl ₃	257.5	1.15	78.5		-1.95	6.26	2.08	5.90	
2,2',4,4'-CBP (PCB47)	C ₁₂ H ₆ Cl ₄	292.0	1.20	41.5		-2.00	6.51	1.88	6.29	
2,2',5,5'-CBP (PCB52)	C ₁₂ H ₆ Cl ₄	292.0	1.20	86.5		-2.30	6.99	1.70	6.09	
3,3',4,4'-CBP (PCB77)	C ₁₂ H ₆ Cl ₄	292.0	1.20	180.0			7.47		6.50	
2,2',3,4,5'-CBP (PCB87)	C ₁₂ H ₅ Cl 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 ₅ Cl 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 ₄ Cl 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 ₃ Cl ₇	395.4		109.5				2.36	7.36	
<i>Miscellaneous Polychlorinated Compounds</i>										
α -hexachlorocyclohexane (α -HCH)	C ₆ H ₆ Cl ₆	290.8		158.0		-2.52	5.28	3.63	3.81	
β -hexachlorocyclohexane (β -HCH)	C ₆ H ₆ Cl ₆	290.8		309.5		-4.40	6.46	4.33	3.80	
γ -hexachlorocyclohexane (lindane, γ -HCH)	C ₆ H ₆ Cl ₆	290.8		112.0		-2.15	4.60	3.94	3.78	
p,p' -DDT	C ₁₄ H ₉ Cl ₅	354.5	1.55	109.0		-4.70	7.80	3.30	6.36	
p,p' -DDE	C ₁₄ H ₈ Cl 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 ₂ H ₆ O	46.1	0.67	-141.5	-24.8	5.77	(1.40 exp.)	0.10
Diethyl ether	C ₄ H ₁₀ O	74.1	0.71	-116.3	34.5	4.85	0.05	0.89
Methyl- <i>t</i> -butyl-ether (MBTE)	C ₅ H ₁₂ O	88.2	0.74	-109.0	55.2	4.51	0.34	0.94
Di- <i>n</i> -propyl ether	C ₆ H ₁₄ O	102.2	0.75	-123.2	90.1	3.92	1.50	2.03
Di-isopropyl ether	C ₆ H ₁₄ O	102.2	0.73	-85.5	68.5	4.30	1.10	1.52
<i>n</i> -Butyl-ethyl ether	C ₆ H ₁₄ O	102.2	0.75	-103.0	92.2	3.90	1.20	2.03
D- <i>n</i> -butyl ether	C ₆ H ₁₈ O	130.2	0.77	-95.2	140.3	2.95	2.75	3.21

Miscellaneous Ethers Including Epoxides

Ethylene oxide (epoxyethane)	C ₂ H ₄ O	44.1	0.87	-111.0	10.7	5.16	-0.93 (1bar)	-0.30
Propyleneoxide (epoxypropane)	C ₃ H ₆ O	58.1	0.83	-112.1	34.2	4.85	-0.91	0.03
Tetrahydrofuran	C ₄ H ₈ O	72.1	0.89	-108.5	66.0	4.33	miscible	0.46
1,4-Dioxane	C ₄ H ₈ O ₂	88.1	1.03	11.0	101.1	3.70	miscible	-0.27
1-Chloro-2,3-epoxypropane (epichlorohydrine)	C ₃ H ₅ ClO	92.5	1.18	-57.2	116.2	3.36	0.15	0.30
Di-2-chloroethyl ether	C ₄ H ₈ Cl ₂ O	143.0	1.22	-46.8	178.0	2.31	1.15	1.29
Methoxybenzene (anisole)	C ₇ H ₈ O	108.2	0.99	-37.5	153.6	2.67	1.80	2.11
Ethoxybenzene (phenetole)	C ₈ H ₁₀ O	122.2	1.07	-31.0	169.5	2.31	2.18	2.51
Styreneoxide	C ₈ H ₈ O	120.2	1.05	-35.6	194.1	1.60	3.16	1.55

*Polychlorinated Dibenzo-*p*-Dioxins (PCDDs), Selected Congeners*

Dibenzo- <i>p</i> -dioxin (DD)	C ₁₂ H ₈ O ₂	184.0		123.0	283.5	-1.26	5.33	4.30
1-CDD	C ₁₂ H ₇ ClO ₂	218.5		105.5	315.5	-1.92	5.72	4.90
2,7-DCDD	C ₁₂ H ₆ Cl ₂ O ₂	253.0		210.0	373.5	-3.92	7.83	5.70
1,2,3,4-TCDD	C ₁₂ H ₄ Cl ₄ O ₂	322.0		190.0	419.0	-5.20	8.77	6.60
2,3,7,8-TCDD	C ₁₂ H ₄ Cl ₄ O ₂	322.0		305.0	446.5	-6.70	10.22	6.80
1,2,3,4,7-PCDD	C ₁₂ H ₃ Cl ₅ O ₂	356.4		196.0	464.7	-7.05	9.48	7.40
1,2,3,4,7,8-HCDD	C ₁₂ H ₂ Cl ₆ O ₂	391.0		273.0	487.7	-8.29	10.94	7.80
Octachloro-DD	C ₁₂ Cl ₈ O ₂	460.0		322.0	510.0	-10.00	12.79	8.20

Polychlorinated Dibenzofurans (PCDFs), Selected Congeners

Dibenzofuran (DF)	C ₁₂ H ₈ O	168.2		86.5	287.0	-0.52	4.55	4.31
2,8-DCDF	C ₁₂ H ₆ Cl ₂ O	237.1		184.0	375.0	-3.41	7.21	5.44
2,3,7,8-TCDF	C ₁₂ H ₄ Cl ₄ O	306.0		227.0	438.0	-5.70	8.86	6.10
2,3,4,7,8-PCDF	C ₁₂ H ₃ Cl ₅ O	340.4		196.0	464.7	-6.46	9.16	6.50
1,2,3,4,7,8-HCDF	C ₁₂ H ₂ Cl ₆ O	374.9		225.5	487.7	-7.50	10.66	7.00
Octachloro-DF	C ₁₂ Cl ₈ O ₂	443.8		258.0	537.0	-9.30	11.58	8.00

Compound Name	Molecular Formula	M_f (g·mol ⁻¹)	ρ_f (g·cm ⁻³)	T_m (°C)	T_b (°C)	$\log p_i^*/\text{Pa}$	$-\log C_{f/w}^{\text{sat}}$	$-\log K_{f/w}$ calculated (experimental)	$\log K_{f/w}$	pK_a
<i>Alkylated Phenols</i>										
Phenol	C ₆ H ₆ O	94.1	1.05	40.9	181.8	1.79	0.005	4.59 (4.79 exp.)	1.44	9.95
2-Methylphenol (<i>o</i> -cresol)	C ₇ H ₈ O	108.1	1.05	30.7	191.0	1.60	0.61	4.18 (4.30 exp.)	2.07	10.28
3-Methylphenol (<i>m</i> -cresol)	C ₇ H ₈ O	108.1	1.03	11.9	202.1	1.30	0.67	4.42	1.98	10.05
4-Methylphenol (<i>p</i> -cresol)	C ₇ H ₈ O	108.1	1.03	35.2	201.9	1.20	0.75	4.44 (4.49 exp.)	1.93	10.25
4-Ethylphenol	C ₈ H ₁₀ O	122.2	1.03	47.0	219.0	0.80	1.18	4.40	2.50	10.00
2,6-Dimethylphenol	C ₈ H 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 ₈ H ₁₀ O	122.2	1.14	67.0		-0.07	1.40	5.06	2.23	10.34
2,4,6-Trimethylphenol	C ₉ H ₁₂ O	136.2		72.0		0.82	2.10	3.47	2.73	10.90
4- <i>n</i> -Butylphenol	C ₁₀ H ₁₄ O	150.2	0.98	22.0	248.0		2.31		3.64	
4- <i>t</i> -Butylphenol	C ₁₀ H ₁₄ O	150.2		99.0	238.0	0.08	2.11	4.20	3.14	9.90
4- <i>n</i> -Octylphenol	C ₁₄ H ₂₂ O	206.3		41.5		-1.14	4.18	3.35		
4- <i>n</i> -Nonylphenol	C ₁₅ H ₂₄ O	220.4	1.51	96.0	295.0	-1.15	4.64	2.89	5.76	
<i>Chlorinated Phenols</i>										
2-Chlorophenol	C ₆ H ₅ ClO	128.6	1.26	9.8	175.2	2.50	0.65	3.24	2.19	8.44
3-Chlorophenol	C ₆ H ₅ ClO	128.6	1.25	32.6	214.0	1.54	0.69	4.16	2.48	8.98
4-Chlorophenol	C ₆ H ₅ ClO	128.6	1.31	42.7	219.0	1.27	0.68	4.43	2.42	9.29
2,4-Dichlorophenol	C ₆ H ₄ Cl ₂ O	163.0	1.38	43.7	213.0	1.20	1.57	3.61	3.09	7.85
2,4,5-Trichlorophenol	C ₆ H ₃ Cl ₃ O	197.5	1.50	62.5		0.62	2.22	3.55	3.90	6.91
2,4,6-Trichlorophenol	C ₆ H ₃ Cl ₃ O	197.5		68.8	243.5	0.37	2.37	3.65	3.67	6.19
2,3,4,5-Tetrachlorophenol	C ₆ H ₂ Cl ₄ O	231.9		117.0		-1.00	3.15	4.24	4.87	6.35
2,3,4,6-Tetrachlorophenol	C ₆ H ₂ Cl ₄ O	231.9		69.5		-0.55	3.10	3.84	4.45	5.40
Pentachlorophenol	C ₆ HCl ₅ O	266.3		189.3		-2.04	4.15	4.28	5.24	4.83
<i>Nitrophenols</i>										
2-Nitrophenol	C ₆ H ₅ NO 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 ₆ H ₅ NO ₃	139.1		96.5			1.03		2.00	8.36
4-Nitrophenol	C ₆ H ₅ NO ₃	139.1	1.48	114.0		-2.26	0.98	7.66	1.96	7.06
2,4-Dinitrophenol	C ₆ H ₄ N ₂ O ₅	184.1		114.1			2.74		1.66	4.01
2,4-Dinitro-6-methylphenol (dinitro- <i>o</i> -cresol; DNOC)	C ₇ H ₆ N ₂ O ₅	198.1		86.5		-1.14	3.00	4.53	2.12	4.31

Miscellaneous Phenolic Compounds

1,2-Dihydroxybenzene (catechol)	C ₆ H ₆ O 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 ₆ H ₆ O 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 ₆ H ₆ O 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 ₇ H ₈ O 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 ₇ H ₆ Cl ₂ O 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 ₇ H ₅ Cl ₃ O 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 ₇ H ₅ Cl ₃ O ₂	227.5		113.5		-1.49	3.62	4.26	3.74	7.07
Tetrachloro-2-methoxyphenol (tetrachloroguaiacol)	C ₇ H ₄ Cl ₄ O ₂	261.9		121.5		-1.80	4.00	4.19	4.45	6.26

Aldehydes

Methanal (formaldehyde)	CH ₂ O	30.0		-92.0	-21.00	5.72		(4.90 exp.)		
Ethanal (acetaldehyde)	C ₂ H ₄ O	44.1	0.78	-123.0	20.8	5.08		(2.52 exp.)	0.45	
Propanal	C ₃ H ₆ O	58.1	0.87	-80.0	48.0	4.63		(2.50 exp.)	0.59	
<i>n</i> -Butanal (butyraldehyde)	C ₄ H ₈ O	72.1	0.80	-96.4	74.8	4.19	0.01	2.20	0.88	
iso-Butanal (isobutyraldehyde)	C ₄ H ₈ O	72.1		-65.0	64.1	4.36		(2.33 exp.)		
<i>n</i> -Pentanal (valeraldehyde)	C ₅ H ₁₀ O	86.1	0.81	-93.5	103.0	3.66		(2.10 exp.)		
Hexanal	C ₆ H ₁₂ O	100.2	0.85	-56.0	131.0	3.17	1.30	(2.22 exp.)	1.92	1.78
2-Propenal (acrolein)	C ₃ H ₄ O	56.1	0.84	-87.3	52.6	4.56		(2.06 exp.)		
Benzaldehyde	C ₇ H ₆ O	106.1	1.04	-26.0	178.8	2.24	1.55	(2.27 exp.)	-0.01	
								2.60	1.48	
								(2.95 exp.)		

Ketones

Propanone (acetone)	C ₃ H ₆ O	58.1	0.79	-94.7	56.1	4.50	miscible	(2.80 exp.)	-0.24	
Butanone	C ₄ H ₈ O	72.1	0.81	-87.0	79.6	4.09		(2.60 exp.)	0.29	
2-Pentanone	C ₅ H ₁₀ O	86.1	0.81	-76.9	102.3	3.70	0.16	2.53	0.90	
2-Hexanone	C ₆ H ₁₂ O	100.2	0.81	-55.8	128.6	3.20	0.76	(2.58 exp.)	1.38	
Cyclohexanone	C ₆ H ₁₀ O	98.1	0.95	-32.1	155.6	2.78	0.63	2.98	0.71	
Methyl-phenyl-ketone (acetophenone)	C ₈ H ₈ O	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)	$\log p^*/Pa$	$-\log C_{iW}^{sat}$	$-\log K_{iW}^{calculated}$ (experimental)	$\log K_{iW}^{exp}$	pK_{iA}
<i>Carboxylic Acids</i>										
Acetic acid	C ₂ H ₄ O ₂	60.1		16.7	117.9					
Propanoic acid	C ₃ H ₆ O ₂	74.1	0.99	-20.7	141.1	3.32	miscible	(4.95 exp.)	-0.25	4.75
Butanoic acid (butyric acid)	C ₄ H ₈ O ₂	88.1	0.96	-5.7	163.7	2.70	miscible	(4.74 exp.)	0.33	4.87
Hexanoic acid	C ₆ H ₁₂ O ₂	116.1	0.93	-3.5	205.0	2.18	0.19	4.02	0.79	4.85
Benzoic acid	C ₇ H ₆ O ₂	122.1	1.27	122.4	249.2	0.70		(4.66 exp.)		
Phenylacetic acid	C ₈ H ₈ O ₂	136.2		77.0	265.0	-0.96	1.55	5.80	1.89	4.19
Salicylic acid	C ₇ H ₆ O ₃	138.1	1.44	159.0	211.0	-0.08	0.92	5.55	1.41	4.31
(2-hydroxy benzoic acid)						-1.70	1.78	5.31	2.24	2.97
<i>o</i> -Phthalic acid	C ₈ H ₆ O ₄	166.1		210.0			1.38			13.40
<i>Carboxylic Acid Esters</i>										
Methyl acetate	C ₃ H ₆ O ₂	74.1	0.93	-98.1	56.9	4.46	-0.52	2.45	0.20	
Ethyl acetate	C ₄ H ₈ O ₂	88.1	0.90	-41.5	77.1	4.10	-0.04	(2.04 exp.)	0.69	
Propyl acetate	C ₅ H ₁₀ O ₂	102.1	0.89	-95.0	101.5	3.65	0.67	(2.16 exp.)	1.24	
Butyl acetate	C ₆ H ₁₂ O ₂	116.2	0.88	-73.5	126.1	3.20	1.28	2.07	1.80	
Hexyl acetate	C ₈ H ₁₆ O ₂	144.2	0.88	-80.9	171.5	2.27	2.46	(2.05 exp.)		
Vinyl acetate	C ₄ H ₆ O ₂	86.1	0.93	-92.8	72.5	4.15	0.64	1.91	2.83	
Methyl benzoate	C ₈ H ₈ O ₂	136.2	1.09	-12.1	199.5	1.72	1.81	1.66	0.73	
Ethyl benzoate	C ₉ H ₁₀ O ₂	150.2	1.05	-34.0	212.4	1.38	2.63	1.60	2.20	
<i>Phthalates</i>										
Dimethylphthalate	C ₁₀ H ₁₀ O ₄	194.2	1.19	5.5	283.7	0.38	1.66	2.86	2.64	
Diethylphthalate	C ₁₂ H ₁₄ O ₄	222.2	1.23	-40.5	296.0	-0.66	2.44	2.38		
Di- <i>n</i> -propyl-phthalate	C ₁₄ H ₁₈ O ₄	250.3			304.5		3.36	4.35	1.53	
Di- <i>n</i> -butyl-phthalate	C ₁₆ H ₂₂ O ₄	278.3	1.05	-35.0	340.0	-2.28	4.36	4.61	2.39	
Benzyl- <i>n</i> -butyl-phthalate	C ₁₉ H ₂₀ O ₄	312.4	1.12	<-35.0	370.0	-2.94	5.08	4.31	3.27	
Di-(2-ethylhexyl)-phthalate	C ₂₄ H ₃₈ O ₄	390.6	0.98	-50.0	385.0	-2.72	7.13	4.25	4.91	
<i>Aromatic Amines</i>										
Aminobenzene (aniline)	C ₆ H ₇ N	93.1	1.01	-6.3	184.4	1.92	0.44	1.98	7.48	
2-Methylaniline (<i>o</i> -toluidine)	C ₇ H ₉ N	107.2	1.00	-16.3	200.3	1.55	0.82	4.03	0.95	4.63
								4.02	1.32	4.44

3-Methylaniline (<i>m</i> -toluidine)	C ₇ H ₉ N	107.2	0.99	-31.5	203.3	1.42	0.85	4.12	1.40	4.72
4-Methylaniline (<i>p</i> -toluidine)	C ₇ H ₉ N	107.2	1.04	43.7	200.4	1.60	1.15	3.64	1.39	5.17
2,6-Dimethylaniline	C ₈ H ₁₁ N	121.2	0.98	11.2	214.0	1.30	1.41	3.68	1.84	3.95
3,4-Dimethylaniline	C ₈ H ₁₁ N	121.2		51.0	228.0		1.65		1.84	5.28
N,N-Dimethylaniline	C ₈ H ₁₁ N	121.2		2.5	194.0	1.95	2.04	2.40	2.31	5.12
2-Chloroaniline	C ₆ H ₆ ClN	127.6	1.21	-14.0	208.8	1.54	1.53	3.32	1.88	2.65
3-Chloroaniline	C ₆ H ₆ ClN	127.6	1.22	-10.3	229.5	0.98	1.37	4.04	1.99	3.52
4-Chloroaniline	C ₆ H ₆ ClN	127.6	1.43	71.0	231.3	0.40	1.64	4.35	1.83	4.00
3,4-Dichloroaniline	C ₆ H ₅ Cl ₂ N	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 ₉ N	143.2	1.13	49.5	300.9		1.92	5.34	2.25	3.92
2-Naphthylamine	C ₁₀ H ₉ N	143.2	1.06	111.5	306.0			5.48	2.30	4.15
<i>Aliphatic Amines</i>										
Methylamine	CH ₅ N	31.1		-92.5	-6.5	5.55		(3.34 exp.)	-0.57	
Dimethylamine	C ₂ H ₇ N	45.1		-96.0	7.4	5.31		(3.15 exp.)	-0.38	10.80
Trimethylamine	C ₃ H ₉ N	59.1		-117.2	2.9	5.34		(2.56 exp.)	0.27	9.80
Ethylamine	C ₂ H ₇ N	45.1		-81.0	16.6	5.15		(3.30 exp.)	-0.13	10.80
Diethylamine	C ₄ H ₁₁ N	73.1	0.71	-49.5	56.1	4.50		(2.98 exp.)	0.50	10.90
<i>n</i> -Propylamine	C ₃ H ₉ N	59.1	0.72	-83.0	48.7	4.62		(3.22 exp.)	0.32	10.70
<i>n</i> -Butylamine	C ₄ H ₁₁ N	73.1	0.74	-50.0	77.9	4.11		(3.11 exp.)	0.98	10.70
<i>n</i> -Hexylamine	C ₆ H ₁₅ N	101.2	0.77	-22.9	132.8	3.07	0.25	3.07	2.06	
								(2.90 exp.)		
<i>Heterocyclic N-Compounds</i>										
Pyridine	C ₅ H ₅ N	79.1	0.98	-41.6	115.3	3.44		(3.44 exp.)	0.65	5.25
2-Methylpyridine (2-picoline)	C ₆ H ₇ N	93.1	0.94	-66.7	129.4	3.18		(3.40 exp.)	1.11	5.97
3-Methylpyridine (3-picoline)	C ₆ H ₇ N	93.1	0.95	-18.1	144.1	3.12		(3.50 exp.)	1.22	5.67
4-Methylpyridine (4-picoline)	C ₆ H ₇ N	93.1	0.95	3.7	145.4	2.88		(3.62 exp.)	1.22	5.99
2,3-Dimethylpyridine (2,3-lutidine)	C ₇ H ₉ N	107.2	0.94	-15.5	163.5	2.62		(3.54 exp.)	1.65	6.57
2,6-Dimethylpyridine (2,6-lutidine)	C ₇ H ₉ N	107.2	0.92	-6.1	144.1	2.87		(3.37 exp.)	1.68	6.65
Quinoline	C ₉ H ₇ N	129.2	1.10	-14.8	237.1	0.08	1.33	4.98	2.06	4.90
								(4.20 exp.)		5.40
Isoquinoline	C ₉ H ₇ N	129.2	1.10	26.5	243.2					
<i>Nitrobenzenes</i>										
Nitrobenzene	C ₆ H ₅ NO ₂	123.1	1.20	5.7	210.8	1.48	1.79	3.12	1.85	
2-Methylnitrobenzene (2-nitrotoluene)	C ₇ H ₇ NO ₂	137.1	1.16	-9.9	222.0	1.43	2.35	2.61	2.30	

Compound Name	Molecular Formula	M_f (g·mol ⁻¹)	ρ_l (g·cm ⁻³)	T_m (°C)	T_b (°C)	$\log p^*/\text{Pa}$	$-\log C_{f/w}^{\text{sat}}$	$-\log K_{f/w}$ calculated (experimental)	$\log K_{f/w}$	pK_a
3-Methylnitrobenzene (3-nitrotoluene)	C ₇ H ₇ NO ₂	137.1		15.9	232.0	1.28	2.43	2.68	2.43	
4-Methylnitrobenzene (4-nitrotoluene)	C ₇ H ₇ NO ₂	137.1	1.39	51.6	238.3	1.20	2.43	2.76	2.38	
2-Chloronitrobenzene	C ₆ H ₄ ClNO ₂	157.6		33.0	245.3	0.70	2.69	3.00 (2.74 exp.)	2.45	
3-Chloronitrobenzene	C ₆ H ₄ ClNO ₂	157.6		45.0	235.6	0.27	2.73	3.39	2.48	
4-Chloronitrobenzene	C ₆ H ₄ ClNO ₂	157.6		83.3	240.5	0.44	2.92	3.03 (2.66 exp.)	2.50	
1,3-Dinitrobenzene	C ₆ H ₄ N ₂ O ₄	168.1		89.9	301.9	-1.92	2.54	5.77	1.49	
1-Methyl-2,4-dinitrobenzene (2,4-dinitrotoluene)	C ₇ H ₆ N ₂ O 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 ₇ H ₆ N ₂ O ₄	182.1	1.28	65.5		-1.12	3.00	4.51	2.03	
1,3,5-Trinitrobenzene	C ₆ H ₃ N ₃ O 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 ₇ H ₅ N ₃ O ₆	227.1		80.8		-3.07	3.24	6.22 (5.98 exp.)	1.98	
<i>Triazine-, Carbamide-, Carbamate-, and Urea Pesticides</i>										
Simazine	C ₇ H ₁₂ ClN ₅	201.7	1.30	226.0		-5.07	4.55	6.91	2.18	
Atrazine	C ₈ H ₁₀ ClN ₅	215.7	1.19	175.0		-4.40	3.86	6.93	2.65	
Cyanazine	C ₉ H 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 ₉ H ₁₂ N ₂ O	164.2	1.08	135.5			1.63		0.98	
Diuron	C ₉ H ₁₀ Cl ₂ N ₂ O	233.1	1.48	158.5		<-4.0	3.76		2.60	
Isoproturon	C ₁₂ H ₁₈ N ₂ O	206.3	1.16	155.5		<-4.0	3.57		2.50	
<i>Phosphoric- and Thiophosphoric Acid (Thio)Esters</i>										
Tributylphosphate	C ₁₂ H ₂₇ O ₄ P	263.3	0.98	<0		-0.10	2.65	3.84	2.50	
Tri- <i>o</i> -cresylphosphat	C ₂₁ H ₂₁ O ₄ P	368.4	1.21	50		-3.00	5.31	4.08	5.11	
Parathion	C ₁₀ H ₁₄ NO ₃ PS	291.3	1.27	6.1		-3.22	4.30	5.31	3.81	
Methylparathion	C ₈ H ₁₀ NO ₃ PS	263.5	1.36	37.5		-2.70	4.00	5.10	3.00	
Fenthion	C ₁₀ H ₁₅ O ₃ PS ₂	278.3	1.25	7.5		-2.70	3.74	5.35	4.10	
Disulfoton	C ₈ H ₁₉ O ₂ PS ₃	274.4	1.14	<25		-1.80	4.20	4.00	4.02	