

Appendix B - Properties and Toxicities of Organic Solvents

The values in the table below except as noted have been extracted from online and hardbound compilations. Values for relative polarity, eluant strength, threshold limits and vapor pressure have been extracted from: Christian Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Publishers, 3rd ed., 2003.

TABLE 1

<u>Solvent</u>	formula	boiling point (°C)	melting point (°C)	density (g/mL)	solubility in H ₂ O ¹ (g/100g)	relative polarity ²	eluant strength ³	threshold limits ⁴ (ppm)	vapor pressure 20°C (hPa)
acetic acid	C ₂ H ₄ O ₂	118	16.6	1.049	M	0.648	>1	10	15.3
acetone	C ₃ H ₆ O	56.2	-94.3	0.786	M	0.355	0.56	500	240
acetonitrile	C ₂ H ₃ N	81.6	-46	0.786	M	0.460	0.65	20	97
acetyl acetone	C ₅ H ₈ O ₂	140.4	-23	0.975	16	0.571			
2-aminoethanol	C ₂ H ₇ NO	170.9	10.5	1.018	M	0.651		3	0.53
aniline	C ₆ H ₇ N	184.4	-6.0	1.022	3.4	0.420		2	0.4
anisole	C ₇ H ₈ O	153.7	-37.5	0.996	0.10	0.198			
benzene	C ₆ H ₆	80.1	5.5	0.879	0.18	0.111	0.32	0.5	101
benzonitrile	C ₇ H ₅ N	205	-13	0.996	0.2	0.333		10	12
benzyl alcohol	C ₇ H ₈ O	205.4	-15.3	1.042	3.5	0.608			
1-butanol	C ₄ H ₁₀ O	117.6	-89.5	0.81	7.7	0.586		20	6.3
2-butanol	C ₄ H ₁₀ O	99.5	-114.7	0.808	18.1	0.506		100	
<i>i</i>-butanol	C ₄ H ₁₀ O	107.9	-108.2	0.803	8.5	0.552			
2-butanone	C ₄ H ₈ O	79.6	-86.3	0.805	25.6	0.327	0.51	200	105
<i>t</i>-butyl alcohol	C ₄ H ₁₀ O	82.2	25.5	0.786	M	0.389		100	41
carbon disulfide	CS ₂	46.3	-111.6	1.263	0.2	0.065	0.15	10	400
carbon tetrachloride	CCl ₄	76.7	-22.4	1.594	0.08	0.052	0.18	5	120
chlorobenzene	C ₆ H ₅ Cl	132	-45.6	1.106	0.05	0.188	0.30	10	12
chloroform	CHCl ₃	61.2	-63.5	1.498	0.8	0.259		10	210
cyclohexane	C ₆ H ₁₂	80.7	6.6	0.779	0.005	0.006	0.04	100	104
cyclohexanol	C ₆ H ₁₂ O	161.1	25.2	0.962	4.2	0.509		50	1.2
cyclohexanone	C ₆ H ₁₀ O	155.6	-16.4	0.948	2.3	0.281		25	5
di-<i>n</i>-butylphthalate	C ₁₆ H ₂₂ O ₄	340	-35	1.049	0.0011	0.272			
1,1-dichloroethane	C ₂ H ₄ Cl ₂	57.3	-97.0	1.176	0.5	0.269		100	240
1,2-dichloroethane	C ₂ H ₄ Cl ₂	83.5	-35.4	1.235	0.87	0.327			

AppB-2

diethylamine	C ₄ H ₁₁ N	56.3	-48	0.706	M	0.145	0.63	5	260
diethylene glycol	C ₄ H ₁₀ O ₃	245	-10	1.118	M	0.713			0.027
diglyme	C ₆ H ₁₄ O ₃	162	-64	0.945	M	0.244			
dimethoxy-ethane (glyme)	C ₄ H ₁₀ O ₂	85	-58	0.868	M	0.231			
N,N-dimethyl-aniline	C ₈ H ₁₁ N	194.2	2.4	0.956	0.14	0.179			
dimethyl-formamide (DMF)	C ₃ H ₇ NO	153	-61	0.944	M	0.386		10	3.5
dimethyl phthalate	C ₁₀ H ₁₀ O ₄	283.8	1	1.190	0.43	0.309			
dimethyl sulfoxide (DMSO)	C ₂ H ₆ OS	189	18.4	1.092	M	0.444	0.75		
dioxane	C ₄ H ₈ O ₂	101.1	11.8	1.033	M	0.164	0.56	20	41
ethanol	C ₂ H ₆ O	78.5	-114.1	0.789	M	0.654	0.88	100	59
ether	C ₄ H ₁₀ O	34.6	-116.3	0.713	7.5	0.117	0.38	400	587
ethyl acetate	C ₄ H ₈ O ₂	77	-83.6	0.894	8.7	0.228	0.58	400	97
ethyl acetoacetate	C ₆ H ₁₀ O ₃	180.4	-80	1.028	2.9	0.577			
ethyl benzoate	C ₉ H ₁₀ O ₂	213	-34.6	1.047	0.07	0.228			
ethylene glycol	C ₂ H ₆ O ₂	197	-13	1.115	M	0.790	1.11		
glycerin	C ₃ H ₈ O ₃	290	17.8	1.261	M	0.812			
heptane	C ₇ H ₁₆	98	-90.6	0.684	0.0003	0.012		400	48
hexane	C ₆ H ₁₄	69	-95	0.655	0.0014	0.009	0.01	50	160
1-hexanol	C ₆ H ₁₄ O	158	-46.7	0.814	0.59	0.559			
methanol	CH ₄ O	64.6	-98	0.791	M	0.762	0.95	200	128
methyl acetate	C ₃ H ₆ O ₂	56.9	-98.1	0.933	24.4	0.253		200	220
methyl <i>t</i>-butyl ether (MTBE)	C ₅ H ₁₂ O	55.2	-109	0.741	4.8	0.124	0.20		
methylene chloride	CH ₂ Cl ₂	39.8	-96.7	1.326	1.32	0.309	0.42	50	475
1-octanol	C ₈ H ₁₈ O	194.4	-15	0.827	0.096	0.537			
pentane	C ₅ H ₁₂	36.1	-129.7	0.626	0.004	0.009	0.00	600	573
1-pentanol	C ₅ H ₁₂ O	138.0	-78.2	0.814	2.2	0.568			
2-pentanol	C ₅ H ₁₂ O	119.0	-50	0.810	4.5	0.488			
3-pentanol	C ₅ H ₁₂ O	115.3	-8	0.821	5.1	0.463			
2-pentanone	C ₅ H ₁₀ O	102.3	-76.9	0.809	4.3	0.321			
3-pentanone	C ₅ H ₁₂ O	101.7	-39.8	0.814	3.4	0.265		200	

1-propanol	C ₃ H ₈ O	97	-126	0.803	M	0.617	0.82		
2-propanol	C ₃ H ₈ O	82.4	-88.5	0.785	M	0.546	0.82	400	44
pyridine	C ₅ H ₅ N	115.5	-42	0.982	M	0.302	0.71	5	20
tetrahydrofuran (THF)	C ₄ H ₈ O	66	-108.4	0.886	30	0.207	0.57	200	200
toluene	C ₇ H ₈	110.6	-93	0.867	0.05	0.099	0.29	50	29
water	H ₂ O	100.00	0.00	0.998	M	1.000	>>1		
water, heavy	D ₂ O	101.3	4	1.107	M	0.991			
p-xylene	C ₈ H ₁₀	138.3	13.3	0.861	0.02	0.074	0.26	100	15

1 M = miscible.

2 The values for relative polarity are normalized from measurements of solvent shifts of absorption spectra and were extracted from Christian Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, Wiley-VCH Publishers, 3rd ed., 2003.

3 Snyder's empirical eluant strength parameter for alumina. Extracted from Reichardt, page 495.

4 Threshold limits for exposure. Extracted from Reichardt, pages 501-502.

TABLE 2

<u>Solvent</u>	formula	boiling point (°C)	melting point (°C)	density (g/mL)	solubility in H ₂ O ¹ (g/100g)	relative polarity ²	eluant strength ³	threshold limits ⁴ (ppm)	vapor pressure 20°C (hPa)
cyclohexane	C ₆ H ₁₂	80.7	6.6	0.779	0.005	0.006	0.04	100	104
pentane	C ₅ H ₁₂	36.1	-129.7	0.626	0.0039	0.009	0.00	600	573
hexane	C ₆ H ₁₄	69	-95	0.655	0.0014	0.009	0.01	50	160
heptane	C ₇ H ₁₆	98	-90.6	0.684	0.0003	0.012		400	48
carbon tetrachloride	CCl ₄	76.7	-22.4	1.594	0.08	0.052	0.18	5	120
carbon disulfide	CS ₂	46.3	-111.6	1.263	0.2	0.065	0.15	10	400
p-xylene	C ₈ H ₁₀	138.3	13.3	0.861	0.02	0.074	0.26	100	15
toluene	C ₇ H ₈	110.6	-93	0.867	0.05	0.099	0.24	50	29
benzene	C ₆ H ₆	80.1	5.5	0.879	0.18	0.111	0.32	0.5	101
ether	C ₄ H ₁₀ O	34.6	-116.3	0.713	7.5	0.117	0.38	400	587
methyl t-butyl ether (MTBE)	C ₅ H ₁₂ O	55.2	-109	0.741	4.8	0.124	0.20		
diethylamine	C ₄ H ₁₁ N	56.3	-48	0.706	M	0.145	0.63	5	260
dioxane	C ₄ H ₈ O ₂	101.1	11.8	1.033	M	0.164	0.56	20	41
N,N-dimethyl-aniline	C ₈ H ₁₁ N	194.2	2.4	0.956	0.14	0.179			
chlorobenzene	C ₆ H ₅ Cl	132	-45.6	1.106	0.05	0.188	0.30	10	12
anisole	C ₇ H ₈ O	153.7	-37.5	0.996	0.10	0.198			
tetrahydrofuran (THF)	C ₄ H ₈ O	66	-108.4	0.886	30	0.207	0.57	200	200

AppB-4

ethyl acetate	C ₄ H ₈ O ₂	77	-83.6	0.894	8.7	0.228	0.57	400	97
ethyl benzoate	C ₉ H ₁₀ O ₂	213	-34.6	1.047	0.07	0.228			
dimethoxy-ethane (glyme)	C ₄ H ₁₀ O ₂	85	-58	0.868	M	0.231			
diglyme	C ₆ H ₁₄ O ₃	162	-64	0.945	M	0.244			
methyl acetate	C ₃ H ₆ O ₂	56.9	-98.1	0.933	24.4	0.253		200	220
chloroform	CHCl ₃	61.2	-63.5	1.498	0.8	0.259	0.40	10	210
3-pentanone	C ₅ H ₁₂ O	101.7	-39.8	0.814	3.4	0.265		200	
1,1-dichloroethane	C ₂ H ₄ Cl ₂	57.3	-97.0	1.176	0.5	0.269		100	240
di-n-butyl phthalate	C ₁₆ H ₂₂ O ₄	340	-35	1.049	0.0011	0.272			
cyclohexanone	C ₆ H ₁₀ O	155.6	-16.4	0.948	2.3	0.281		25	5
pyridine	C ₅ H ₅ N	115.5	-42	0.982	M	0.302	0.71	5	20
dimethylphthalate	C ₁₀ H ₁₀ O ₄	283.8	1	1.190	0.43	0.309			
methylene chloride	CH ₂ Cl ₂	39.8	-96.7	1.326	1.32	0.309	0.42	50	475
2-pentanone	C ₅ H ₁₀ O	102.3	-76.9	0.809	4.3	0.321			
2-butanone	C ₄ H ₈ O	79.6	-86.3	0.805	25.6	0.327	0.51	200	105
1,2-dichloroethane	C ₂ H ₄ Cl ₂	83.5	-35.4	1.235	0.87	0.327			
benzonitrile	C ₇ H ₅ N	205	-13	0.996	0.2	0.333		10	12
acetone	C ₃ H ₆ O	56.2	-94.3	0.786	M	0.355	0.56	500	240
dimethyl-formamide (DMF)	C ₃ H ₇ NO	153	-61	0.944	M	0.386		10	3.5
<i>t</i> -butyl alcohol	C ₄ H ₁₀ O	82.2	25.5	0.786	M	0.389		100	41
aniline	C ₆ H ₇ N	184.4	-6.0	1.022	3.4	0.420		2	0.4
dimethyl sulfoxide (DMSO)	C ₂ H ₆ OS	189	18.4	1.092	M	0.444	0.75		
acetonitrile	C ₂ H ₃ N	81.6	-46	0.786	M	0.460	0.65	20	97
3-pentanol	C ₅ H ₁₂ O	115.3	-8	0.821	5.1	0.463			
2-pentanol	C ₅ H ₁₂ O	119.0	-50	0.810	4.5	0.488			
2-butanol	C ₄ H ₁₀ O	99.5	-114.7	0.808	18.1	0.506		100	
cyclohexanol	C ₆ H ₁₂ O	161.1	25.2	0.962	4.2	0.509		50	1.2
1-octanol	C ₈ H ₁₈ O	194.4	-15	0.827	0.096	0.537			
2-propanol	C ₃ H ₈ O	82.4	-88.5	0.785	M	0.546	0.82	400	44
<i>i</i> -butanol	C ₄ H ₁₀ O	107.9	-108.2	0.803	8.5	0.552			
1-hexanol	C ₆ H ₁₄ O	158	-46.7	0.814	0.59	0.559			

1-pentanol	$C_5H_{12}O$	138.0	-78.2	0.814	2.2	0.568			
acetyl acetone	$C_5H_8O_2$	140.4	-23	0.975	16	0.571			
ethyl acetoacetate	$C_6H_{10}O_3$	180.4	-80	1.028	2.9	0.577			
1-butanol	$C_4H_{10}O$	117.6	-89.5	0.81	7.7	0.586		20	6.3
benzyl alcohol	C_7H_8O	205.4	-15.3	1.042	3.5	0.608			
1-propanol	C_3H_8O	97	-126	0.803	M	0.617	0.82		
acetic acid	$C_2H_4O_2$	118	16.6	1.049	M	0.648	>1	10	15.3
2-aminoethanol	C_2H_7NO	170.9	10.5	1.018	M	0.651		3	0.53
ethanol	C_2H_6O	78.5	-114.1	0.789	M	0.654	0.88	1000	59
diethylene glycol	$C_4H_{10}O_3$	245	-10	1.118	M	0.713			0.027
methanol	CH_4O	64.6	-98	0.791	M	0.762	0.95	200	128
ethylene glycol	$C_2H_6O_2$	197	-13	1.115	M	0.790	1.11		
glycerin	$C_3H_8O_3$	290	17.8	1.261	M	0.812			
water, heavy	D_2O	101.3	4	1.107	M	0.991			
water	H_2O	100.00	0.00	0.998	M	1.000	>>1		