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

Solvent	formula	boiling point (°C)	melting point (°C)	density (g/mL)	solubility in H_2O[1] (g/100g)	relative polarity[2]	eluant strength[3]	threshold limits[4] (ppm)	vapor pressure 20°C (hPa)
acetic acid	$C_2H_4O_2$	118	16.6	1.049	M	0.648	>1	10	15.3
acetone	C_3H_6O	56.2	-94.3	0.786	M	0.355	0.56	500	240
acetonitrile	C_2H_3N	81.6	-46	0.786	M	0.460	0.65	20	97
acetyl acetone	$C_5H_8O_2$	140.4	-23	0.975	16	0.571			
2-aminoethanol	C_2H_7NO	170.9	10.5	1.018	M	0.651		3	0.53
aniline	C_6H_7N	184.4	-6.0	1.022	3.4	0.420		2	0.4
anisole	C_7H_8O	153.7	-37.5	0.996	0.10	0.198			
benzene	C_6H_6	80.1	5.5	0.879	0.18	0.111	0.32	0.5	101
benzonitrile	C_7H_5N	205	-13	0.996	0.2	0.333		10	12
benzyl alcohol	C_7H_8O	205.4	-15.3	1.042	3.5	0.608			
1-butanol	$C_4H_{10}O$	117.6	-89.5	0.81	7.7	0.586		20	6.3
2-butanol	$C_4H_{10}O$	99.5	-114.7	0.808	18.1	0.506		100	
***i*-butanol**	$C_4H_{10}O$	107.9	-108.2	0.803	8.5	0.552			
2-butanone	C_4H_8O	79.6	-86.3	0.805	25.6	0.327	0.51	200	105
***t*-butyl alcohol**	$C_4H_{10}O$	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_6H_5Cl	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_6H_{12}	80.7	6.6	0.779	0.005	0.006	0.04	100	104
cyclohexanol	$C_6H_{12}O$	161.1	25.2	0.962	4.2	0.509		50	1.2
cyclohexanone	$C_6H_{10}O$	155.6	-16.4	0.948	2.3	0.281		25	5
di-n-butylphthalate	$C_{16}H_{22}O_4$	340	-35	1.049	0.0011	0.272			
1,1-dichloroethane	$C_2H_4Cl_2$	57.3	-97.0	1.176	0.5	0.269		100	240
1,2-dichloroethane	$C_2H_4Cl_2$	83.5	-35.4	1.235	0.87	0.327			

diethylamine	$C_4H_{11}N$	56.3	-48	0.706	M	0.145	0.63	5	260
diethylene glycol	$C_4H_{10}O_3$	245	-10	1.118	M	0.713			0.027
diglyme	$C_6H_{14}O_3$	162	-64	0.945	M	0.244			
dimethoxy-ethane (glyme)	$C_4H_{10}O_2$	85	-58	0.868	M	0.231			
N,N-dimethyl-aniline	$C_8H_{11}N$	194.2	2.4	0.956	0.14	0.179			
dimethyl-formamide (DMF)	C_3H_7NO	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_2H_6OS	189	18.4	1.092	M	0.444	0.75		
dioxane	$C_4H_8O_2$	101.1	11.8	1.033	M	0.164	0.56	20	41
ethanol	C_2H_6O	78.5	-114.1	0.789	M	0.654	0.88	100	59
ether	$C_4H_{10}O$	34.6	-116.3	0.713	7.5	0.117	0.38	400	587
ethyl acetate	$C_4H_8O_2$	77	-83.6	0.894	8.7	0.228	0.58	400	97
ethyl acetoacetate	$C_6H_{10}O_3$	180.4	-80	1.028	2.9	0.577			
ethyl benzoate	$C_9H_{10}O_2$	213	-34.6	1.047	0.07	0.228			
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			
heptane	C_7H_{16}	98	-90.6	0.684	0.0003	0.012		400	48
hexane	C_6H_{14}	69	-95	0.655	0.0014	0.009	0.01	50	160
1-hexanol	$C_6H_{14}O$	158	-46.7	0.814	0.59	0.559			
methanol	CH_4O	64.6	-98	0.791	M	0.762	0.95	200	128
methyl acetate	$C_3H_6O_2$	56.9	-98.1	0.933	24.4	0.253		200	220
methyl *t*-butyl ether (MTBE)	$C_5H_{12}O$	55.2	-109	0.741	4.8	0.124	0.20		
methylene chloride	CH_2Cl_2	39.8	-96.7	1.326	1.32	0.309	0.42	50	475
1-octanol	$C_8H_{18}O$	194.4	-15	0.827	0.096	0.537			
pentane	C_5H_{12}	36.1	-129.7	0.626	0.004	0.009	0.00	600	573
1-pentanol	$C_5H_{12}O$	138.0	-78.2	0.814	2.2	0.568			
2-pentanol	$C_5H_{12}O$	119.0	-50	0.810	4.5	0.488			
3-pentanol	$C_5H_{12}O$	115.3	-8	0.821	5.1	0.463			
2-pentanone	$C_5H_{10}O$	102.3	-76.9	0.809	4.3	0.321			
3-pentanone	$C_5H_{12}O$	101.7	-39.8	0.814	3.4	0.265		200	

1-propanol	C_3H_8O	97	-126	0.803	M	0.617	0.82		
2-propanol	C_3H_8O	82.4	-88.5	0.785	M	0.546	0.82	400	44
pyridine	C_5H_5N	115.5	-42	0.982	M	0.302	0.71	5	20
tetrahydrofuran (THF)	C_4H_8O	66	-108.4	0.886	30	0.207	0.57	200	200
toluene	C_7H_8	110.6	-93	0.867	0.05	0.099	0.29	50	29
water	H_2O	100.00	0.00	0.998	M	1.000	>>1		
water, heavy	D_2O	101.3	4	1.107	M	0.991			
***p*-xylene**	C_8H_{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

Solvent	formula	boiling point (°C)	melting point (°C)	density (g/mL)	solubility in H_2O[1] (g/100g)	**relative polarity**[2]	eluant strength[3]	threshold limits[4] (ppm)	vapor pressure 20°C (hPa)
cyclohexane	C_6H_{12}	80.7	6.6	0.779	0.005	**0.006**	0.04	100	104
pentane	C_5H_{12}	36.1	-129.7	0.626	0.0039	**0.009**	0.00	600	573
hexane	C_6H_{14}	69	-95	0.655	0.0014	**0.009**	0.01	50	160
heptane	C_7H_{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_8H_{10}	138.3	13.3	0.861	0.02	**0.074**	0.26	100	15
toluene	C_7H_8	110.6	-93	0.867	0.05	**0.099**	0.24	50	29
benzene	C_6H_6	80.1	5.5	0.879	0.18	**0.111**	0.32	0.5	101
ether	$C_4H_{10}O$	34.6	-116.3	0.713	7.5	**0.117**	0.38	400	587
methyl *t*-butyl ether (MTBE)	$C_5H_{12}O$	55.2	-109	0.741	4.8	**0.124**	0.20		
diethylamine	$C_4H_{11}N$	56.3	-48	0.706	M	**0.145**	0.63	5	260
dioxane	$C_4H_8O_2$	101.1	11.8	1.033	M	**0.164**	0.56	20	41
N,N-dimethyl-aniline	$C_8H_{11}N$	194.2	2.4	0.956	0.14	**0.179**			
chlorobenzene	C_6H_5Cl	132	-45.6	1.106	0.05	**0.188**	0.30	10	12
anisole	C_7H_8O	153.7	-37.5	0.996	0.10	**0.198**			
tetrahydrofuran (THF)	C_4H_8O	66	-108.4	0.886	30	**0.207**	0.57	200	200

ethyl acetate	$C_4H_8O_2$	77	-83.6	0.894	8.7	**0.228**	0.57	400	97
ethyl benzoate	$C_9H_{10}O_2$	213	-34.6	1.047	0.07	**0.228**			
dimethoxy-ethane (glyme)	$C_4H_{10}O_2$	85	-58	0.868	M	**0.231**			
diglyme	$C_6H_{14}O_3$	162	-64	0.945	M	**0.244**			
methyl acetate	$C_3H_6O_2$	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	$C_5H_{12}O$	101.7	-39.8	0.814	3.4	**0.265**		200	
1,1-dichloroethane	$C_2H_4Cl_2$	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	$C_6H_{10}O$	155.6	-16.4	0.948	2.3	**0.281**		25	5
pyridine	C_5H_5N	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_2Cl_2	39.8	-96.7	1.326	1.32	**0.309**	0.42	50	475
2-pentanone	$C_5H_{10}O$	102.3	-76.9	0.809	4.3	**0.321**			
2-butanone	C_4H_8O	79.6	-86.3	0.805	25.6	**0.327**	0.51	200	105
1,2-dichloroethane	$C_2H_4Cl_2$	83.5	-35.4	1.235	0.87	**0.327**			
benzonitrile	C_7H_5N	205	-13	0.996	0.2	**0.333**		10	12
acetone	C_3H_6O	56.2	-94.3	0.786	M	**0.355**	0.56	500	240
dimethyl-formamide (DMF)	C_3H_7NO	153	-61	0.944	M	**0.386**		10	3.5
t-butyl alcohol	$C_4H_{10}O$	82.2	25.5	0.786	M	**0.389**		100	41
aniline	C_6H_7N	184.4	-6.0	1.022	3.4	**0.420**		2	0.4
dimethyl sulfoxide (DMSO)	C_2H_6OS	189	18.4	1.092	M	**0.444**	0.75		
acetonitrile	C_2H_3N	81.6	-46	0.786	M	**0.460**	0.65	20	97
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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**			
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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		