1. **Solvent Polarity Table**
2. **pKa Compilation**
3. **NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities**

Properties 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**.
For **Spectra of Solvents**, jump to the bottom of this p http://murov.info/webercises.htm age. For an ***Organic Chemistry Directory***, see: http://murov.info/orgchem.htm .
For a **Chemistry Directory**, see: http://murov.info/webercises.htm
For much more complete information on physical and safety properties of solvents, please go to:
http://www.knovel.com/web/portal/browse/display?_EXT_KNOVEL_DISPLAY_bookid=761
http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
The tables below were posted (10/23/98) and revised (07/28/09) and updated (04/10/10) by Steve Murov, Professor Emeritus of Chemistry.

Table 1 arranged alphabetically, **Table 2 arranged according to increasing polarity**

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 pressur 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
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			
dimethoxyethane (glyme)	$C_4H_{10}O_2$	85	-58	0.868	M	0.231			
N,N-dimethylaniline	$C_8H_{11}N$	194.2	2.4	0.956	0.14	0.179			
dimethylformamide (DMF)	C_3H_7NO	153	-61	0.944	M	0.386		10	3.5
dimethylphthalate	$C_{10}H_{10}O_4$	283.8	1	1.190	0.43	0.309			
dimethylsulfoxide (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
1-heptanol	$C_7H_{16}O$	176.4	-35	0.819	0.17	0.549			
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 pressur 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-dimethylaniline	$C_8H_{11}N$	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**			
dimethoxyethane (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
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1-hexanol	$C_6H_{14}O$	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**			
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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		

Spectra (of solvents and other compounds)

1. ir, nmr, mass spectra
   Aldrich - **http://www.sigmaaldrich.com/**
   NIMC site - **http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng**
   RSC - **http://www.rsc.org/education/teachers/learnnet/spectra/index2.htm**

2. ir, mass spectra, uv-vis
   NIST site - **http://webbook.nist.gov/chemistry/**

3. ir
   Acros - **http://www.acros.com/portal/alias__Rainbow/lang__en/tabID__21/DesktopDefault.aspx**
   ChemExper Chem Directory - **http://www.chemexper.com/**

4. nmr
   human metabolites - **http://hmdb.ca/** (also some mass spectra)
   bioorganics - **http://mmcd.nmrfam.wisc.edu/mmcdbrowse.html**
   Solvents - **http://www.alsnotebook.com/chlorformtraces.html**

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