SUPPLEMENTAL MATERIAL

ENTHALPY OF SOLVATION CORRELATIONS FOR GASEOUS SOLUTES DISSOLVED IN ALCOHOL SOLVENTS BASED ON THE ABRAHAM MODEL

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TABLE S1. Values of the gas to methanol solvation enthalpy, $\Delta H_{Solv,MeOH}$, in kJ/mole at 298 K for 188 solutes, together with the solute descriptors

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Obs	Ref
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-3.60	21
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	-7.95	21
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	-13.10	21
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	-16.36	21
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	-18.79	21
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	-22.38	22
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	-26.53	22
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	-30.75	22
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	-34.89	22
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	-38.83	22
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	-42.80	22
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	-51.09	22
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.0812	-59.50	23
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630	-67.99	22
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.9540	-23.26	23
3,3-Diethylpentane	0.000	0.000	0.000	0.000	3.820	1.0949	-37.24	23
2-Methyloctane	0.000	0.000	0.000	0.000	3.966	1.3767	-37.70	23
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	-29.46	23
2,2,4,4-Tetramethylpentane	0.000	0.000	0.000	0.000	3.512	1.3767	-32.30	23
2,2,5,5-Tetramethylhexane	0.000	0.000	0.000	0.000	4.039	1.5176	-34.31	23
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045	-24.60	23
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	-28.11	23
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.1272	-36.90	23
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	-30.29	23
cis-1,2-Dimethylcyclohexane	0.281	0.240	0.000	0.000	3.847	1.1272	-34.35	23
Adamantane	0.760	0.570	0.000	0.040	4.934	1.1918	-42.30	25
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	-19.20	26
cis 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	-20.73	27
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7701	-23.43	23
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	-27.82	23
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.0519	-31.84	23
1-Octene	0.094	0.080	0.000	0.070	3.568	1.1928	-35.81	23
1-Nonene	0.090	0.080	0.000	0.070	4.073	1.3337	-39.96	23

1-Decene	0.090	0.080	0.000	0.070	4.554	1.4746	-44.27	23
1-Dodecene	0.089	0.080	0.000	0.070	5.515	1.7564	-52.59	23
1-Tridecene	0.087	0.080	0.000	0.070	6.020	1.8973	-56.57	23
1-Tetradecene	0.085	0.080	0.000	0.070	6.513	2.0382	-60.88	23
1-Pentadecene	0.083	0.080	0.000	0.070	7.006	2.1791	-65.18	23
cis 2-Octene	0.135	0.080	0.000	0.070	3.683	1.1928	-34.98	23
trans 2-Octene	0.123	0.080	0.000	0.070	3.600	1.1928	-34.94	23
cis 4-Octene	0.133	0.080	0.000	0.070	3.607	1.1928	-34.69	23
trans 4-Octene	0.144	0.080	0.000	0.070	3.593	1.1928	-34.39	23
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	-21.50	26
1,5-Hexadiene	0.191	0.150	0.000	0.100	2.450	0.8680	-29.12	23
Cyclopentene	0.335	0.200	0.000	0.100	2.402	0.6605	-25.44	23
Cyclohexene	0.395	0.200	0.000	0.100	3.021	0.8025	-29.54	23
1-Methylcyclohexene	0.391	0.200	0.000	0.100	3.483	0.9433	-33.85	23
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	-37.80	29
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	-42.30	29
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	-45.86	29
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	-51.15	29
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	-55.33	29
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0170	-59.52	30
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2950	-67.39	29
Decan-1-ol	0.191	0.420	0.370	0.480	5.628	1.5763	-76.49	31
Ethylene glycol	0.404	0.900	0.580	0.780	2.661	0.5078	-64.93	32
1,2-Propanediol	0.373	0.900	0.580	0.800	2.918	0.6487	-64.70	32
1,3-Propanediol	0.397	0.910	0.770	0.850	3.263	0.6487	-71.50	47
1,4-Butanediol	0.395	0.930	0.720	0.900	3.795	0.7896	-76.20	47
Glycerol	0.512	0.760	0.470	1.430	3.973	0.7074	-90.10	47
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	-32.37	33
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	-35.37	36
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	-39.94	28
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391	-42.34	28
4-Isopropyltoluene	0.607	0.490	0.000	0.190	4.590	1.1391	-46.58	28
sec-Butylbenzene	0.603	0.480	0.000	0.160	4.506	1.2800	-46.74	28
tert-Butylbenzene	0.619	0.490	0.000	0.180	4.413	1.2800	-44.63	28
Hexamethylbenzene	0.950	0.720	0.000	0.210	6.557	1.5618	-62.25	28
Octylbenzene	0.579	0.480	0.000	0.150	6.714	1.8436	-60.37	28
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.1391	-46.45	28
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	-53.79	35
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3240	-61.85	28

Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	-36.10	69
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.7391	-32.98	34
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	-23.72	27
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	-27.44	37
2-Methyl-2-bromopropane	0.305	0.290	0.000	0.070	2.609	0.8472	-28.80	38,39
2-Methyl-2-iodopropane	0.589	0.350	0.000	0.190	3.439	0.9304	-32.80	39
Methyl iodide	0.676	0.430	0.000	0.120	2.016	0.5077	-25.95	40
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4248	-18.97	27
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	-28.79	41
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	-32.26	41
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288	-35.86	24
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.8288	-36.02	24
2-Hexanone	0.136	0.680	0.000	0.510	3.286	0.9697	-40.12	24
3-Hexanone	0.136	0.660	0.000	0.510	3.310	0.9697	-39.46	24
2-Heptanone	0.123	0.680	0.000	0.510	3.760	1.1106	-44.31	41
4-Heptanone	0.110	0.660	0.000	0.510	3.705	1.1106	-43.22	41
2-Octanone	0.108	0.680	0.000	0.510	4.257	1.2515	-48.24	24
2-Nonanone	0.119	0.680	0.000	0.510	4.735	1.3924	-51.88	41
5-Nonanone	0.103	0.660	0.000	0.510	4.698	1.3924	-50.96	41
2-Decanone	0.108	0.680	0.000	0.510	5.245	1.5333	-55.27	24
2-Undecanone	0.101	0.680	0.000	0.510	5.732	1.6740	-59.00	24
6-Undecanone	0.083	0.660	0.000	0.510	5.677	1.6740	-57.44	24
4-Methyl-2-pentanone	0.111	0.650	0.000	0.510	3.089	0.9697	-39.63	41
3,3-Dimethyl-2-butanone	0.106	0.620	0.000	0.510	2.928	0.9697	-35.52	24
2,2,4,4-Tetramethyl-3-pentanone	0.099	0.560	0.000	0.520	4.370	1.3924	-41.51	41
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.7200	-39.25	24
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8610	-44.48	41
Cycloheptanone	0.436	0.860	0.000	0.560	4.376	1.0020	-46.65	24
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	-17.70	27
Diisopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.0127	-32.89	42
Butyl methyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	-30.63	52
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	-30.75	53
Methyl *tert*-amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	-34.72	54
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	-30.96	43
Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	-33.48	44
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	-34.82	43
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	-36.50	47
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	-91.28	49, 14
18-Crown-6	0.400	1.340	0.000	2.130	7.919	2.0430	-101.6	50

Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	-59.17	55
Nitric oxide	0.370	0.020	0.000	0.090	-0.590	0.2026	-2.64	56
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	5.86	21
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	4.81	21
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.84	21
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-4.90	21
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	-9.41	57
Radon	0.000	0.000	0.000	0.000	0.877	0.3840	-15.98	21
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	0.50	21
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	0.67	21
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	-10.67	51
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.96	21
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	-29.02	58
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	-31.74	61
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	-28.62	62
Butyronitrile	0.180	0.900	0.000	0.360	2.548	0.6860	-35.87	63
Dimethyl sulfoxide	0.522	1.740	0.000	0.880	3.459	0.6126	-53.89	62
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	-47.80	62
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	-40.19	64
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	-46.28	28
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612	-46.11	68
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	-35.39	28
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	-42.55	28
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.9746	-47.47	28
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	-33.94	65
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	-91.16	45
4-Bromophenol	1.080	1.170	0.670	0.200	5.135	0.9500	-82.82	45
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	-66.02	45
4-Methylphenol	0.820	0.870	0.570	0.310	4.312	0.9160	-66.66	45
4-tert-Butylphenol	0.810	0.890	0.560	0.410	5.264	1.3387	-78.34	45
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	-44.21	48
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162	-48.36	48
4-Methylpyridine	0.630	0.820	0.000	0.540	3.64	0.8162	-50.43	66
4-Ethylpyridine	0.634	0.800	0.000	0.570	4.124	0.7571	-50.80	118
2,6-Dimethylpyridine	0.607	0.700	0.000	0.630	3.76	0.9571	-52.89	48
3,5-Dimethylpyridine	0.659	0.790	0.000	0.600	4.214	0.9571	-54.77	66
3-Chloropyridine	0.732	0.830	0.000	0.400	3.783	0.7977	-49.60	48
4-Cyanopyridine	0.750	1.210	0.000	0.590	4.033	0.8300	-52.00	48
4-Methoxypyridine	0.680	0.930	0.000	0.530	4.279	0.8750	-56.57	66

Ethyl benzoate	0.689	0.850	0.000	0.460	5.075	1.2140	-53.93	67
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	-50.84	28
1,2-Dinitrobenzene	1.170	1.700	0.000	0.380	5.910	1.0650	-64.05	28
1,4-Dinitrobenzene	1.130	1.630	0.000	0.460	5.796	1.0650	-70.25	28
1-Chloro-2-nitrobenzene	1.020	1.240	0.000	0.240	5.235	1.0130	-61.15	28
1-Chloro-3-nitrobenzene	1.000	1.140	0.000	0.250	5.206	1.0130	-57.87	28
1-Chloro-4-nitrobenzene	0.980	1.180	0.000	0.240	5.220	1.0130	-57.12	28
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0140	-48.37	28
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	-53.22	28
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	-88.06	28
Anisole	0.710	0.750	0.000	0.290	3.890	0.9160	-43.26	52
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8710	-48.70	28
3-Methylaniline	0.966	0.920	0.230	0.450	4.463	0.9571	-60.94	28
2-Nitroaniline	1.180	1.370	0.300	0.360	5.627	0.9904	-71.42	28
3-Nitroaniline	1.200	1.710	0.400	0.350	5.880	0.9904	-78.09	28
4-Nitroaniline	1.220	1.930	0.460	0.350	6.343	0.9904	-86.44	28
1,2-Diphenylethane	1.200	1.030	0.000	0.280	6.764	1.6060	-66.71	28
N,N-Dimethylaniline	0.957	0.810	0.000	0.410	4.701	1.0980	-48.52	28
1-Chloronaphthalene	1.417	1.000	0.000	0.140	5.856	1.2078	-61.70	28
1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2596	-72.90	28
1-Naphthylamine	1.670	1.200	0.200	0.570	6.490	1.1850	-78.49	28
Styrene	0.849	0.650	0.000	0.160	3.856	0.9552	-42.04	28
alpha-Methylstyrene	0.851	0.640	0.000	0.190	4.290	1.0960	-46.47	28
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	-74.91	28
Diphenyl ether	1.216	1.080	0.000	0.200	6.287	1.3830	-62.34	28
Trifluorotoluene	0.225	0.480	0.000	0.100	2.894	0.9104	-37.78	52
1-Naphthol	1.520	1.050	0.600	0.370	6.130	1.1441	-83.47	70
Quinoline	1.268	0.970	0.000	0.540	5.457	1.0440	-60.33	68
Pyrrole	0.613	0.730	0.410	0.290	2.865	0.5770	-46.48	46
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	-37.32	46
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	-78.66	59,60
2,2,2-Trifluoroethanol	0.015	0.600	0.570	0.250	1.224	0.5022	-47.10	72
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1210	-58.11	73
Benzamide	0.990	1.500	0.490	0.670	5.767	0.9728	-85.05	71
Benzoic acid	0.730	0.900	0.590	0.400	4.510	0.9317	-77.03	71
Picric acid	1.430	2.660	0.460	0.420	8.128	1.2977	-95.57	156
Tetramethylsilicon	-0.057	0.080	0.000	0.000	1.812	0.9179	-20.90	74
Tetraethyltin	0.464	0.180	0.000	0.130	4.923	1.6067	-42.82	155

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Solute	**E**	**S**	**A**	**B**	**L**	**V**	Obs	Ref
Methane	0.000	0.000	0.000	0.000	-0.323	0.2945	-3.85	51
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Propane	0.000	0.000	0.000	0.000	1.050	0.5313	-14.06	21
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	-20.56	81
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	-20.09	81
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	-24.97	92
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	-28.83	77
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	-33.46	97
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	-34.35	98
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	-47.32	99
Undecane	0.000	0.000	0.000	0.000	5.191	1.6585	-50.59	77
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630	-73.59	100
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	-32.28	78
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045	-26.52	101
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	-30.24	102
Adamantane	0.760	0.570	0.000	0.040	4.934	1.1920	-45.02	25
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	-37.40	92
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	-42.30	29
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	-46.18	29
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	-51.82	29
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	-55.65	29
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0170	-60.00	75
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2950	-69.35	29
Decan-1-ol	0.191	0.420	0.370	0.480	5.628	1.5763	-78.91	76
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	-45.46	103
Ethylene glycol	0.404	0.900	0.580	0.780	2.661	0.5078	-63.36	104
1,2-Propanediol	0.373	0.900	0.580	0.800	2.918	0.6487	-69.84	32
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	-16.37	105
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	-25.63	86
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2950	-41.99	87
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	-30.37	88
Diisopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.0127	-31.95	42
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.8718	-29.36	107
Methyl *tert*-amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	-34.61	99, 43
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	-30.44	108

Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	-32.58	115
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	-32.99	106
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	-34.73	109
1,2-Diethoxyethane	0.008	0.730	0.000	0.790	3.310	1.0704	-41.78	85
2-Methyl-2-bromopropane	0.305	0.290	0.000	0.070	2.609	0.8472	-30.06	38
2-Methyl-2-chloropropane	0.142	0.300	0.000	0.030	2.273	0.7946	-27.48	39
2-Methyl-2-iodopropane	0.589	0.350	0.000	0.190	3.439	0.9304	-33.61	39
Nitric oxide	0.370	0.020	0.000	0.090	-0.590	0.2026	-4.52	56
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	7.23	51
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	3.90	51
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.38	51
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	-9.44	57
Radon	0.000	0.000	0.000	0.000	0.877	0.3840	-11.88	21
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	3.72	51
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	0.46	51
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-1.21	51
Carbon Monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	0.33	51
Carbon Dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	-12.80	51
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	-32.01	65
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	-55.34	38
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	-44.00	110
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.6644	-30.39	111
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	-37.85	89
alpha-Methylstyrene	0.851	0.640	0.000	0.190	4.290	1.0960	-47.11	112
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	-26.20	97
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	-30.83	79
4-Methyl-2-pentanone	0.111	0.650	0.000	0.510	3.089	0.9697	-37.76	79
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8610	-41.00	113
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	-57.25	114
Ethyl formate	0.146	0.660	0.000	0.380	1.845	0.6057	-27.62	116
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	-27.86	117
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	-30.44	61
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	-34.61	117
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	-38.83	82
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	-44.20	83
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	-30.53	84
Methyl butanoate	0.106	0.600	0.000	0.450	2.893	0.8875	-35.99	84
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	-38.21	84
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	-27.14	120

Butyronitrile	0.188	0.900	0.000	0.360	2.548	0.6860	-33.87	121
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.7391	-33.19	122
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	-36.90	69
Dimethyl sulfoxide	0.522	1.740	0.000	0.880	3.459	0.6126	-49.19	119
Piperidine	0.422	0.460	0.100	0.690	3.304	0.8043	-53.89	80
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	-47.31	80
Benzylamine	0.829	0.880	0.100	0.720	4.385	0.9570	-59.50	80
Morpholine	0.434	0.790	0.060	0.910	3.289	0.7221	-52.15	80
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	-43.42	80
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162	-46.89	80
4-Ethylpyridine	0.634	0.800	0.000	0.570	4.124	0.9571	-48.80	118
3-Chloropyridine	0.732	0.830	0.000	0.400	3.783	0.7977	-46.30	118
Quinoline	1.268	0.970	0.000	0.540	5.457	1.0440	-60.07	80
2,2,2-Trifluoroethanol	0.015	0.600	0.570	0.250	1.224	0.5022	-48.20	72
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	-32.17	92
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	-35.40	36
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	-40.48	92
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982	-39.93	94
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	-40.67	92
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1210	-52.65	73
Ammonia	0.139	0.390	0.160	0.560	0.319	0.2084	-26.23	96
Difluoromethane	-0.320	0.490	0.060	0.050	0.040	0.2849	-11.53	90
Dichlorodifluoromethane	0.037	0.040	0.000	0.040	0.998	0.5297	-17.64	90
Chlorodifluoromethane	0.000	0.250	0.200	0.000	0.690	0.4073	-15.82	90
Pentafluoroethane	-0.510	-0.019	0.105	0.064	0.100	0.4789	-16.542	90
1,1,1,2-Tetrafluoroethane	-0.390	0.160	0.160	0.050	0.403	0.4612	-15.14	90
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	-15.14	90
Chloropentafluoroethane	-0.360	-0.100	0.000	0.000	0.543	0.6013	-12.55	90
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	-52.40	91
Imidazole	0.710	0.850	0.420	0.780	4.018	0.5360	-73.48	95
N,N-Dimethylformamide	0.367	1.310	0.000	0.740	3.173	0.6468	-44.77	123
2,4,4-Trimethyl-1-pentene	0.090	0.070	0.000	0.070	3.289	1.1928	-33.13	124
Benzamide	0.990	1.500	0.490	0.670	5.767	0.9728	-82.75	71
Benzoic acid	0.730	0.900	0.590	0.400	4.510	0.9317	-76.53	71
Tetramethylsilicon	-0.057	0.080	0.000	0.000	1.812	0.9179	-22.2	74
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	-45.53	125
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	-36.30	93

TABLE S3. Values of the gas to 1-butanol solvation enthalpy, $\Delta H_{Solv,BtOH}$, in kJ/mole at 298 K for 103 solutes, together with the solute descriptors

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Obs	Ref
Methane	0.000	0.000	0.000	0.000	-0.323	0.2945	-3.77	21
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	-12.14	126
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	-17.7	21
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	-17.87	127
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	-25.69	92
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	-30.17	92
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	-34.81	92
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	-39.21	77
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	-42.55	85
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	-48.38	130
Undecane	0.000	0.000	0.000	0.000	5.191	1.6585	-54.03	129
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994	-56.66	85
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.0810	-67.94	130
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630	-76.64	130
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	-33.69	78
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045	-30.54	21
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	-31.60	130
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	-32.98	132
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	-10.42	126
Propene	0.103	0.080	0.000	0.070	0.946	0.4883	-14.12	127
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	-18.50	127
iso-Butene	0.120	0.080	0.000	0.080	1.579	0.6292	-18.40	127
cis-2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	-21.48	128
trans-2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	-19.84	127
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	-19.20	127
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	-26.03	133
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	-37.80	92
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	-42.30	92
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	-46.30	92
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	-52.10	92
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	-56.69	92
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0170	-60.38	92
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2950	-70.24	134
Decan-1-ol	0.191	0.420	0.370	0.480	5.628	1.5763	-80.45	135
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	-17.80	128

Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	-24.01	133
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.8718	-30.37	143
Diisopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.0127	-31.65	42
2-Methyltetrahydrofuran	0.241	0.480	0.000	0.530	2.82	0.7632	-31.55	145
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	-30.56	146
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	-70.37	144
2,5,8,11,14-pentaoxopentadecane	-0.020	1.110	0.000	1.790	6.498	1.8111	-68.73	147
1-Bromobutane	0.360	0.400	0.000	0.120	3.105	0.9304	-34.08	149
2-Methyl-2-bromopropane	0.305	0.290	0.000	0.070	2.609	0.9304	-29.44	122
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4943	-29.35	133
Chloroform	0.425	0.490	0.150	0.020	2.480	0.6167	-35.50	69
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.7391	-32.63	122
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	-23.45	128
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	-31.65	150
2-Chlorobutane	0.189	0.350	0.000	0.122	2.540	0.7946	-29.61	150
1-Chlorohexane	0.201	0.400	0.000	0.100	3.777	1.0770	-40.48	151
2-Methyl-2-chloropropane	0.142	0.300	0.000	0.030	2.273	0.7946	-26.88	122
Trichloroethene	0.524	0.370	0.080	0.030	2.997	0.7146	-34.05	152
2-Methyl-2-iodopropane	0.589	0.350	0.000	0.190	3.439	0.9304	-32.89	39
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	5.52	126
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	6.53	126
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-2.38	21
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-4.89	126
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	-10.49	126
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.42	21
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-1.63	21
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-1.21	21
Carbon Monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-1.42	21
Carbon Dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	-11.43	126
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-7.78	126
Carbon tetrafluoride	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-1.71	126
1-Bromoadamantane	1.070	0.900	0.000	0.200	6.130	1.3668	-55.75	38
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	-45.4	143
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.6644	-29.81	142
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462	-35.65	141
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	-25.33	133
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	-26.93	133
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	-53.49	131
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	-25.14	136

Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	-28.99	137
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	-33.54	138
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	-37.92	139
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	-42.72	140
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	-29.37	84
Methyl butanoate	0.106	0.600	0.000	0.450	2.893	0.8875	-33.37	84
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	-36.99	84
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	-23.71	153
Butyronitrile	0.188	0.900	0.000	0.360	2.548	0.6860	-32.01	121
Dimethyl sulfoxide	0.522	1.740	0.000	0.880	3.459	0.6126	-46.72	119
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	-45.80	143
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	-40.40	118
4-Ethylpyridine	0.634	0.800	0.000	0.570	4.124	0.9571	-50.90	118
3-Chloropyridine	0.732	0.830	0.000	0.400	3.783	0.7977	-45.30	118
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	-31.34	92
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	-35.86	92
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	-40.11	92
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	-39.63	131
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	-48.54	131
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	-47.47	131
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	-17.25	128
Benzamide	0.990	1.500	0.490	0.670	5.767	0.9728	-81.11	71
Benzoic acid	0.730	0.900	0.590	0.400	4.510	0.9317	-74.65	71
Tetramethylsilicon	-0.057	0.080	0.000	0.030	1.812	0.9179	-23.30	74
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	-43.45	125
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0140	-47.29	148
N-Methylpyrrole	0.559	0.790	0.000	0.310	2.923	0.7180	-35.61	46
beta-Pinene	0.530	0.240	0.000	0.190	4.394	1.2574	-44.68	154