

SUPPORTING MATERIAL FOR
ENTHALPY OF SOLVATION CORRELATIONS FOR GASEOUS SOLUTES
DISSOLVED IN WATER AND IN 1-OCTANOL BASED ON THE ABRAHAM
MODEL

Christina Mintz^a, Michael Clark^b, William E. Acree, Jr.^{a*} and Michael H. Abraham^c

Table S1. Values of the gas to water solvation enthalpy in kJ/mol at 298K for 366 solutes, together with the solute descriptors.

Solute	E	S	A	B	L	V	Exp Value	Ref
Chlorine gas	0.360	0.32	0.10	0.00	1.193	0.3434	-23.40	44
Hydrogen sulfide	0.350	0.31	0.10	0.07	0.723	0.2721	-18.00	44
Hydrogen selenide	0.500	0.30	0.03	0.09	1.060	0.3211	-15.70	44
Chlorine dioxide	0.100	0.46	0.00	0.30	0.550	0.3269	-27.80	44
Sulphur hexafluoride	-0.600	-0.20	0.00	0.00	-0.120	0.4643	-20.70	25
Ammonia	0.139	0.39	0.16	0.56	0.319	0.2984	-35.40	44
Methane	0.000	0.00	0.00	0.00	-0.323	0.2495	-12.00	25
Ethane	0.000	0.00	0.00	0.00	0.492	0.3904	-17.90	25
Propane	0.000	0.00	0.00	0.00	1.050	0.5313	-20.40	25
Butane	0.000	0.00	0.00	0.00	1.615	0.6722	-24.80	25
2-Methylpropane	0.000	0.00	0.00	0.00	1.409	0.6722	-21.70	25
Pentane	0.000	0.00	0.00	0.00	2.162	0.8131	-28.30	22
2,2-Dimethylpropane	0.000	0.00	0.00	0.00	1.820	0.8131	-23.40	25
Hexane	0.000	0.00	0.00	0.00	2.668	0.9540	-31.90	25
2-Methylpentane	0.000	0.00	0.00	0.00	2.503	0.9540	-30.50	25
3-Methylpentane	0.000	0.00	0.00	0.00	2.581	0.9540	-36.80	25
2,3-Dimethylbutane	0.000	0.00	0.00	0.00	2.495	0.9540	-32.40	25
Heptane	0.000	0.00	0.00	0.00	3.173	1.0949	-34.00	22
Octane	0.000	0.00	0.00	0.00	3.677	1.2358	-36.00	22
2,2,4-Trimethylpentane	0.000	0.00	0.00	0.00	3.106	1.2358	-31.00	25
2,3,4-Trimethylpentane	0.000	0.00	0.00	0.00	3.481	1.2358	-38.50	25
Cyclopropane	0.408	0.23	0.00	0.00	1.314	0.4227	-15.40	25
Cyclopentane	0.263	0.10	0.00	0.00	2.477	0.7045	-30.33	22
Cyclohexane	0.305	0.10	0.00	0.00	2.964	0.8454	-30.00	25
cis-1,2-Dimethylcyclohexane	0.281	0.24	0.00	0.00	3.847	1.1272	-38.30	25
trans-1,2-Dimethylcyclohexane	0.227	0.20	0.00	0.00	3.728	1.1272	-36.10	25
Ethylcyclohexane	0.263	0.10	0.00	0.00	3.877	1.1272	-36.80	25
Cyclooctane	0.413	0.10	0.00	0.00	4.329	1.1272	-39.00	25
Ethene	0.107	0.10	0.00	0.07	0.289	0.3474	-13.70	25
Propene	0.103	0.08	0.00	0.07	0.946	0.4883	-21.60	22
1-Butene	0.100	0.08	0.00	0.07	1.491	0.6292	-24.10	22
1-Hexene	0.078	0.080	0.000	0.07	2.572	0.9110	-30.40	25
1-Octene	0.094	0.080	0.000	0.07	3.568	1.1928	-39.20	44
2-Methylpropene	0.120	0.08	0.00	0.08	1.579	0.6292	-22.70	25
2-Methyl-2-butene	0.063	0.06	0.00	0.05	1.933	0.7701	-26.61	66
1,3-Butadiene	0.320	0.23	0.00	0.10	1.543	0.5862	-31.40	25
Cyclohexene	0.395	0.200	0.000	0.100	3.021	0.8025	-27.30	25
Cyclooctene	0.460	0.240	0.000	0.100	4.119	1.0842	-45.50	25
Propyne	0.180	0.250	0.120	0.100	1.025	0.4453	-15.60	25

1-Butyne	0.180	0.250	0.120	0.100	1.025	0.5862	-13.50	25
Fluoromethane	0.066	0.35	0.00	0.09	0.057	0.2672	-16.10	25
Difluoromethane	-0.320	0.49	0.06	0.05	0.040	0.3026	-17.20	25
Tetrafluoromethane	-0.580	-0.26	0.00	0.00	-0.817	0.3202	-13.50	25
1,1-Difluoroethane	-0.250	0.47	0.04	0.07	0.570	0.4258	-20.70	25
Trifluoromethane	-0.427	0.183	0.11	0.034	-0.274	0.3026	-22.60	25
1,1,1,2-Tetrafluoroethane	-0.390	0.16	0.16	0.05	0.403	0.4612	-22.20	25
Pentafluoroethane	-0.510	-0.019	0.105	0.064	0.100	0.4789	-21.50	25
1,1,1,2,3,3,3-Heptafluoropropane	-0.690	0.05	0.06	0.03	0.645	0.6552	-24.80	25
Chloromethane	0.249	0.43	0.00	0.08	1.163	0.3719	-20.20	25
Dichloromethane	0.387	0.57	0.10	0.05	2.019	0.4943	-30.30	25
Trichloromethane	0.425	0.49	0.15	0.02	2.480	0.6167	-33.50	25
Tetrachloromethane	0.458	0.38	0.00	0.00	2.823	0.7391	-30.50	46
Chloroethane	0.227	0.40	0.00	0.10	1.678	0.5128	-22.00	25
1,1-Dichloroethane	0.322	0.49	0.10	0.10	2.316	0.6352	-30.30	25
1,2-Dichloroethane	0.416	0.64	0.10	0.11	2.573	0.6352	-27.90	25
1,1,1-Trichloroethane	0.369	0.41	0.00	0.09	2.733	0.7576	-28.70	25
1,1,2-Trichloroethane	0.499	0.68	0.13	0.13	3.290	0.7576	-32.50	25
1,1,2,2-Tetrachloroethane	0.595	0.76	0.16	0.12	3.803	0.8800	-34.80	25
1,1,1,2-Tetrachloroethane	0.542	0.63	0.10	0.08	3.641	0.8800	-36.20	25
1-Chloropropane	0.216	0.40	0.00	0.10	2.202	0.6537	-27.00	25
1,2-Dichloropropane	0.369	0.63	0.00	0.17	2.836	0.7761	-31.10	25
1,3-Dichloropropane	0.408	0.74	0.00	0.17	3.101	0.7761	-29.70	25
1-Chlorobutane	0.210	0.40	0.00	0.10	2.722	0.7946	-28.20	25
2-Chlorobutane	0.189	0.35	0.00	0.12	2.540	0.7955	-34.60	25
1-Chloropentane	0.208	0.38	0.00	0.09	3.223	0.9355	-34.10	25
1-Chlorohexane	0.201	0.40	0.00	0.10	3.777	1.0770	-34.50	25
Tetrafluoroethene	-0.310	-0.10	0.00	0.00	-0.050	0.4182	-15.10	25
Hexafluoropropene	-0.500	-0.10	0.00	0.10	0.337	0.5945	-17.40	25
1,1-Dichloroethylene	0.362	0.34	0.00	0.05	2.110	0.5922	-28.50	25
cis-1,2-Dichloroethylene	0.436	0.61	0.11	0.05	2.439	0.5922	-26.90	56
trans-1,2-Dichloroethylene	0.425	0.41	0.09	0.05	2.278	0.5922	-29.30	56
Trichloroethylene	0.524	0.37	0.08	0.03	2.997	0.7146	-32.20	25
Tetrachloroethylene	0.639	0.44	0.00	0.00	3.584	0.8370	-41.50*	44
Bromomethane	0.399	0.43	0.00	0.10	1.630	0.4243	-23.80	25
Dibromomethane	0.714	0.69	0.11	0.07	2.886	0.5995	-33.00	25
Tribromomethane	0.974	0.68	0.15	0.06	3.784	0.7745	-35.80	44
Bromoethane	0.366	0.40	0.00	0.12	2.120	0.5654	-29.50	25
2-Methyl-2-bromopropane	0.305	0.29	0.00	0.07	2.609	0.8472	-25.40	22
Iodomethane	0.676	0.43	0.00	0.12	2.106	0.5077	-28.20	25
Diiodomethane	1.200	0.69	0.05	0.17	3.857	0.7659	-41.60	44
Iodoethane	0.640	0.40	0.00	0.15	2.573	0.6486	-31.70	25
1-Iodopropane	0.634	0.40	0.00	0.14	3.130	0.7895	-35.30	25
2-Iodopropane	0.622	0.35	0.00	0.17	2.900	0.7895	-36.60	25
Fluorochloromethane	0.042	0.61	0.07	0.04	0.982	0.3896	-21.70	44
Difluorochloromethane	0.000	0.25	0.20	0.00	0.690	0.4073	-22.80	25

Bromodichloromethane	0.593	0.69	0.10	0.04	2.891	0.6693	-28.90	25
Chlorodibromomethane	0.775	0.68	0.12	0.10	3.304	0.7219	-33.30	44
Fluorotrichloromethane	0.207	0.24	0.00	0.07	1.950	0.6344	-19.80	44
Difluorodichloromethane	0.037	0.13	0.00	0.00	1.124	0.5297	-26.00	44
1,1,2-Trichlorotrifluoroethane	0.010	0.13	0.00	0.00	2.210	0.8107	-28.80	25
1,2-Dichlorotetrafluoroethane	-0.190	0.05	0.00	0.00	1.427	0.7060	-20.20	25
Dimethyl ether	0.000	0.27	0.00	0.41	1.285	0.4491	-34.00	26
Diethyl ether	0.041	0.25	0.00	0.45	2.015	0.7309	-45.30	25
Di-n-propyl ether	0.008	0.25	0.00	0.45	2.954	1.0127	-49.90	26
Di-isopropyl ether	-0.060	0.16	0.00	0.58	2.530	1.0127	-51.70	26
Dibutyl ether	0.000	0.25	0.00	0.45	3.924	1.2950	-55.80	25
Methyl propyl ether	0.060	0.25	0.00	0.45	2.090	0.7309	-38.00	26
Ethyl butyl ether	0.013	0.25	0.00	0.45	2.989	1.0170	-48.40	26
Methyl tert-butyl ether	0.024	0.21	0.00	0.59	2.380	0.8718	-48.70	26
Ethyl tert-butyl ether	-0.020	0.16	0.00	0.60	2.720	1.0127	-53.40	26
Methyl tert-pentyl ether	0.050	0.21	0.00	0.60	2.916	1.0127	-52.50	26
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	-47.30	26
2,5-Dimethyltetrahydrofuran	0.204	0.380	0.000	0.580	2.980	0.9041	-56.30	24
2-Methyltetrahydrofuran	0.241	0.480	0.000	0.530	2.820	0.7632	-51.40	24
Tetrahydropyran	0.275	0.470	0.000	0.550	3.057	0.7672	-48.90	24
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	-48.40	25
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	-59.30	24
1,2-Diethoxyethane	0.008	0.730	0.000	0.790	3.310	1.0714	-71.90	24
1-Methoxy-2-ethoxyethane	0.060	0.700	0.000	0.740	2.982	0.9305	-66.10	26
1-Methoxy-2-propoxyethane	0.010	0.730	0.000	0.790	3.310	1.0714	-69.10	26
1,2-Dipropoxyethane	0.000	0.640	0.000	0.780	4.386	1.3532	-76.80	26
3,6,9-Trioxoundecane	0.040	0.870	0.000	1.200	4.815	1.4119	-96.20	26
2,5,8,11-Tetraoxododecane	0.000	0.980	0.000	1.440	5.157	1.4706	-102.40	26
2,5,8,11,14-Pentaoxopentadecane	-0.020	1.110	0.000	1.790	6.498	1.8111	-125.80	26
Methoxyflurane	0.109	0.670	0.07	0.140	2.864	0.8700	-30.40	25
Isoflurane	-0.240	0.500	0.10	0.100	1.902	0.8009	-35.30	25
Propanone	0.179	0.700	0.04	0.490	1.696	0.5470	-39.70	25
Butanone	0.166	0.700	0.00	0.510	2.287	0.6879	-41.90	25
Pentan-2-one	0.143	0.680	0.00	0.510	2.755	0.8288	-45.31	34
Pentan-3-one	0.154	0.660	0.00	0.510	2.811	0.8288	-49.45	29
Hexan-2-one	0.136	0.680	0.00	0.510	3.286	0.9697	-48.90	25
4-Methylpentan-2-one	0.111	0.650	0.00	0.510	3.089	0.9697	-44.60	25
Methyl isopropyl ketone	0.134	0.650	0.00	0.510	2.692	0.8288	-57.60	25
3,3-Dimethyl-2-butanone	0.106	0.620	0.000	0.510	2.928	0.9697	-47.50	30
Diisopropyl ketone	0.072	0.600	0.000	0.510	3.403	1.1106	-54.00	30
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	-54.90	25
Heptan-4-one	0.110	0.660	0.000	0.510	3.705	1.1106	-58.10	30
Octan-2-one	0.108	0.680	0.000	0.510	4.257	1.2515	-58.30	25
Nonan-5-one	0.103	0.660	0.000	0.510	4.698	1.3924	-62.80	25
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.7200	-44.30	25

Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8610	-49.80	25
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0140	-53.30	25
Propiophenone	0.804	0.950	0.000	0.510	4.971	1.1550	-61.90	25
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	-38.10	25
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	-40.80	25
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	-48.70	29
Isopropyl acetate	0.055	0.570	0.000	0.470	2.546	0.8875	-46.80	29
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	-52.70	29,35
Isobutyl acetate	0.052	0.570	0.000	0.470	3.161	1.0284	-51.80	29
sec-Butyl acetate	0.044	0.570	0.000	0.470	3.054	1.0284	-47.99	35
tert-Butyl acetate	0.025	0.540	0.000	0.470	2.802	1.0284	-42.60	29
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	-55.34	29
Isopentyl acetate	0.051	0.570	0.000	0.470	3.740	1.1693	-53.80	29
Hexyl acetate	0.056	0.600	0.000	0.450	4.351	1.3102	-60.80	29
Methyl formate	0.192	0.680	0.000	0.380	1.285	0.4648	-32.70	29
Ethyl formate	0.146	0.660	0.000	0.380	1.845	0.6057	-38.10	29
Propyl formate	0.132	0.630	0.000	0.380	2.433	0.7466	-40.51	29
Isopropyl formate	0.091	0.600	0.000	0.400	2.230	0.7466	-43.00	29
Isobutyl formate	0.095	0.600	0.000	0.400	2.789	0.8875	-43.00	29
Pentyl formate	0.101	0.630	0.000	0.380	3.488	1.0284	-48.10	29
3-Methylbutyl formate	0.092	0.600	0.000	0.400	3.306	1.0284	-47.70	29
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	-44.50	29
Ethyl propanoate	0.087	0.580	0.000	0.450	2.807	0.8875	-49.50	29
Propyl propanoate	0.070	0.560	0.000	0.450	3.338	1.0284	-51.20	29
Butyl propanoate	0.058	0.560	0.000	0.470	3.833	1.1693	-57.80	29
Isobutyl propanoate	0.032	0.530	0.000	0.470	3.635	1.1693	-54.70	29
Methyl butanoate	0.106	0.600	0.000	0.450	2.893	0.8875	-47.50	29
Ethyl butanoate	0.068	0.580	0.000	0.450	3.271	1.0284	-52.70	29
Propyl butanoate	0.050	0.560	0.000	0.450	3.783	1.1693	-54.90	29
Butyl butanoate	0.044	0.560	0.000	0.450	4.275	1.3102	-63.50	29
Methyl 2-methylpropanoate	0.087	0.570	0.000	0.470	2.636	0.8875	-46.00	29
Ethyl 2-methylpropanoate	0.034	0.550	0.000	0.470	3.072	1.0284	-51.30	29
Isobutyl 2-methylpropanoate	0.000	0.500	0.000	0.470	3.885	1.3102	-55.30	29
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	-50.40	29
Ethyl pentanoate	0.049	0.580	0.000	0.450	3.769	1.1693	-56.50	29
Methyl 2,2-dimethylpropanoate	0.049	0.540	0.000	0.450	2.932	1.0284	-46.20	29
Ethyl 2,2-dimethylpropanoate	-0.010	0.520	0.000	0.450	3.481	1.1693	-50.30	29
Ethyl 3-methylbutanoate	0.025	0.550	0.000	0.470	3.579	1.1693	-56.00	29
Ethyl 2-methylbutanoate	0.026	0.550	0.000	0.470	3.565	1.1693	-55.40	29
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	-54.70	29
Ethyl hexanoate	0.043	0.580	0.000	0.450	4.251	1.3102	-60.20	29
Methyl benzoate	0.733	0.850	0.000	0.460	4.704	1.0730	-50.25	22
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	-35.70	22
Nitroethane	0.270	0.950	0.020	0.330	2.414	0.5646	-32.50	25
1-Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055	-34.40	25
2-Nitropropane	0.216	0.920	0.000	0.330	2.550	0.7055	-34.10	25

Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	-52.00	36
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	-50.60	25
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	-59.90	25
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	-58.20	57
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	-61.90	25
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7309	-62.72	61
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	-60.20	24,22
tert-Butanol	0.180	0.300	0.310	0.600	1.963	0.7309	-62.90	61
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	-61.90	25
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	-66.00	24
2-Pentanol	0.195	0.360	0.330	0.560	2.840	0.8718	-63.30	25
3-Pentanol	0.195	0.360	0.330	0.560	2.860	0.8718	-59.60	25
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0170	-67.40	25
Hexan-3-ol	0.200	0.360	0.330	0.560	3.440	1.0170	-69.60	24
2-Methyl-2-butanol	0.194	0.300	0.310	0.600	2.630	0.8718	-68.44	38
4-Methyl-2-pentanol	0.167	0.330	0.330	0.560	3.179	1.0127	-69.90	25
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.1536	-72.13	22
Heptane-2-ol	0.188	0.360	0.330	0.560	3.842	1.1536	-72.60	58
Heptan-4-ol	0.180	0.360	0.330	0.560	3.850	1.1536	-75.30	24
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2950	-74.14	22
Dodecan-1-ol	0.175	0.420	0.370	0.480	6.640	1.8580	-81.90	55
Cyclopentanol	0.427	0.540	0.320	0.560	3.241	0.7630	-58.50	25
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.9040	-70.70	39
Cycloheptanol	0.513	0.540	0.320	0.580	4.407	1.0450	-74.60	22
Ethan-1,2-diol	0.404	0.900	0.580	0.780	2.661	0.5078	-77.30	24
Propan-1,3-diol	0.397	0.910	0.770	0.850	3.263	0.6487	-81.10	60
Butan-1,4-diol	0.395	0.930	0.720	0.900	3.795	0.7896	-89.60	60
Glycerol	0.512	0.760	0.470	1.430	3.973	0.7074	-103.50	24
2-Methoxyethanol	0.269	0.500	0.300	0.840	2.490	0.6487	-60.40	24
2-Ethoxyethanol	0.237	0.520	0.310	0.810	2.792	0.7896	-66.40	24
2-Propoxyethanol	0.212	0.500	0.300	0.830	3.310	0.9305	-69.60	24
2-Butoxyethanol	0.201	0.500	0.300	0.830	3.806	1.0714	-73.60	24
Benzene	0.610	0.520	0.000	0.140	2.786	0.7176	-28.10	25
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	-32.40	25
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	-39.40	25
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	-37.70	22
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	-38.60	25
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	-34.80	25
Propylbenzene	0.604	0.500	0.000	0.150	4.230	1.1391	-36.40	25
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391	-33.70	25
1,2,3-Trimethylbenzene	0.728	0.610	0.000	0.190	4.565	1.1391	-37.36	22
1,2,4-Trimethylbenzene	0.677	0.560	0.000	0.190	4.441	1.1391	-36.60	25
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.1391	-39.12	22
4-Isopropyltoluene	0.607	0.490	0.000	0.190	4.590	1.2800	-34.60	25
Butylbenzene	0.600	0.510	0.000	0.150	4.730	1.2800	-38.50	25
Pentylbenzene	0.594	0.510	0.000	0.150	5.230	1.4210	-49.45	22

Hexylbenzene	0.591	0.500	0.000	0.150	5.720	1.5618	-52.72	22
1,4-Diethylbenzene	0.645	0.500	0.000	0.180	4.732	1.2800	-46.40	25
Styrene	0.849	0.650	0.000	0.160	3.856	0.9552	-28.40	25
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	-29.30	25
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	-30.60	25
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	-37.30	25
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.9612	-35.30	25
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612	-28.40	25
1,2,3-Trichlorobenzene	1.030	0.860	0.000	0.000	5.419	1.0836	-32.60	25
1,3,5-Trichlorobenzene	0.980	0.730	0.000	0.000	5.045	1.0836	-34.20	25
1,2,3,4-Tetrachlorobenzene	1.180	0.920	0.000	0.000	6.171	1.2060	-35.00	25
Pentachlorobenzene	1.330	0.960	0.000	0.000	6.716	1.3280	-39.90	25
2-Chlorotoluene	0.762	0.650	0.000	0.070	4.173	0.9797	-38.30	25
3-Chlorotoluene	0.736	0.670	0.000	0.070	4.179	0.9797	-37.00	25
4-Chlorotoluene	0.705	0.740	0.000	0.050	4.205	0.9797	-33.30	25
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	-33.50	25
Phenyl methyl ether	0.708	0.750	0.000	0.290	3.890	0.9160	-41.42	22
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	-56.50	25
2-Ethylaniline	0.962	0.850	0.230	0.450	4.829	1.0980	-59.70	25
4-Ethylaniline	0.942	0.910	0.230	0.450	4.895	1.0980	-65.00	25
2,4-Dimethylaniline	0.950	0.950	0.200	0.490	4.983	1.0980	-58.70	25
2,5-Dimethylaniline	0.962	0.930	0.200	0.480	4.966	1.0980	-61.50	25
2,6-Dimethylaniline	0.972	0.900	0.050	0.590	5.028	1.0980	-60.50	25
N,N-Dimethylaniline	0.957	0.810	0.000	0.410	4.701	1.0980	-49.60	25
N,N-Diethylaniline	0.953	0.800	0.000	0.410	5.287	1.0980	-45.70	25
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	-43.80	25
2-Nitrotoluene	0.866	1.110	0.000	0.270	4.878	1.0320	-46.40	25
3-Nitrotoluene	0.874	1.100	0.000	0.250	5.097	1.0320	-38.50	25
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	-57.70	41
2-Methylphenol	0.840	0.860	0.520	0.300	4.218	0.9160	-64.80	25
3-Methylphenol	0.822	0.880	0.570	0.340	4.310	0.9160	-58.70	24
4-Methylphenol	0.820	0.870	0.570	0.310	4.312	0.9160	-61.30	24
4-tert-Butylphenol	0.810	0.890	0.560	0.410	5.264	1.3387	-63.80	24
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	-50.30	24
3-Cyanophenol	0.930	1.550	0.770	0.280	5.184	0.9298	-70.70	24
4-Cyanophenol	0.930	1.550	0.770	0.280	5.184	0.9298	-70.30	24
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	-49.80	25
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	-67.70	24
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	-68.60	24
Biphenyl (approx)	1.360	0.990	0.000	0.260	6.014	1.3240	-47.20	25
Naphthalene (approx)	1.340	0.920	0.000	0.200	5.161	1.0854	-42.80	25
1-Methylnaphthalene	1.337	0.940	0.000	0.220	5.802	1.2260	-45.00	25
2-Methylnaphthalene	1.304	0.810	0.000	0.250	5.617	1.2260	-44.90	25
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	-52.10	25
Fluorene	1.588	1.060	0.000	0.250	6.922	1.3570	-42.70	25
Propanal	0.196	0.650	0.000	0.450	1.815	0.5470	-39.40	25

Pentanal	0.163	0.650	0.000	0.450	2.770	0.8288	-42.90	25
Hexanal	0.146	0.650	0.000	0.450	3.370	0.9697	-55.20	25
Heptanal	0.140	0.650	0.000	0.450	3.860	1.1106	-56.60	25
Octanal	0.160	0.650	0.000	0.450	4.380	1.2515	-48.80	25
Isobutyl aldehyde	0.144	0.620	0.000	0.450	2.120	0.6879	-40.00	25
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	-42.10	25
3-Hydroxybenzaldehyde	0.990	1.380	0.730	0.400	5.060	0.9317	-70.70	24
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	-34.80	27
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5451	-39.52	27
Butyronitrile	0.180	0.900	0.000	0.360	2.548	0.6860	-42.10	27
Pentanenitrile	0.177	0.900	0.000	0.360	3.108	0.8269	-45.60	27
2-Cyanopropane	0.140	0.870	0.000	0.400	2.465	0.6860	-40.00	27
1,2-Dicyanoethane	0.350	2.100	0.000	0.500	3.918	0.6998	-58.20	27
1,3-Dicyanopropane	0.330	2.050	0.000	0.590	4.342	0.8407	-63.50	27
1,4-Dicyanobutane	0.320	2.080	0.000	0.620	4.853	0.9816	-66.60	27
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8710	-48.50	22
2,2,2-Trifluoroethanol	0.015	0.600	0.570	0.250	1.224	0.5022	-50.20	22
1,1,1-Trifluoropropan-2-ol	0.105	0.470	0.370	0.360	1.963	0.6431	-53.50	24
2,2,3,3-Tetrafluoropropan-1-ol	0.006	0.440	0.770	0.180	1.949	0.6608	-57.90	24
2,2,3,3,3-Pentafluoropropan-1-ol	-0.170	0.330	0.620	0.170	1.598	0.6785	-51.90	24
1,1,1,3,3,3-Hexafluoropropan-2-ol	-0.240	0.550	0.770	0.100	1.392	0.6962	-57.10	24
Methylamine	0.250	0.350	0.160	0.580	1.300	0.3493	-45.27	22
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	-53.68	22
Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	-55.98	22
Isopropylamine	0.181	0.320	0.160	0.610	1.908	0.6311	-55.00	24
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	-59.20	22
sec-Butylamine	0.170	0.320	0.160	0.630	2.410	0.7720	-57.10	24
tert-Butylamine	0.121	0.290	0.160	0.710	2.493	0.7720	-59.00	24
Pentylamine	0.211	0.350	0.160	0.610	3.139	0.9129	-62.13	22,24
Hexylamine	0.197	0.350	0.160	0.610	3.655	1.0538	-65.93	22,24
Octylamine	0.187	0.350	0.160	0.610	4.520	1.3350	-52.3*	25
Dimethylamine	0.189	0.300	0.080	0.660	1.600	0.4902	-53.09	22
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	-64.30	22
Dipropylamine	0.124	0.300	0.080	0.690	3.351	1.0538	-65.20	25
Dibutylamine	0.107	0.300	0.080	0.690	4.349	1.3356	-59.30	25
Trimethylamine	0.140	0.200	0.000	0.670	1.620	0.6310	-52.71	22
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	-69.70	24
1,2-Diaminoethane	0.462	0.170	0.040	1.290	1.880	0.5900	-76.10	24
1,3-Diaminopropane	0.446	0.610	0.430	1.140	2.852	0.7309	-85.60	24
1,4-Diaminobutane	0.431	0.620	0.420	1.140	3.367	0.8718	-91.60	24
1,5-Diaminopentane	0.422	0.630	0.390	1.150	3.895	1.0127	-95.10	24
Piperidine	0.422	0.460	0.100	0.690	3.304	0.8043	-65.41	24
N-Methylpiperidine	0.318	0.340	0.000	0.720	3.330	0.9452	-65.77	24
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	-42.10	25
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162	-50.30	25
3-Methylpyridine	0.631	0.810	0.000	0.540	3.631	0.8162	-50.30	25

4-Methylpyridine	0.630	0.820	0.000	0.540	3.640	0.8162	-51.80	25
2-Ethylpyridine	0.613	0.710	0.000	0.590	3.844	0.9571	-55.70	24
3-Ethylpyridine	0.640	0.790	0.000	0.570	4.093	0.9571	-53.50	24
4-Ethylpyridine	0.634	0.800	0.000	0.570	4.124	0.9571	-52.20	24
2,3-Dimethylpyridine	0.657	0.770	0.000	0.620	4.045	0.9571	-57.70	24
2,4-Dimethylpyridine	0.634	0.760	0.000	0.630	4.006	0.9571	-60.70	24
2,5-Dimethylpyridine	0.633	0.740	0.000	0.620	3.986	0.9571	-54.90	24
2,6-Dimethylpyridine	0.607	0.700	0.000	0.630	3.760	0.9571	-52.30	25
3,4-Dimethylpyridine	0.676	0.850	0.000	0.620	4.317	0.9571	-50.50	25
3,5-Dimethylpyridine	0.659	0.790	0.000	0.600	4.214	0.9571	-51.30	25
2-Chloropyridine	0.738	1.030	0.000	0.370	3.875	0.7977	-42.56	54
3-Chloropyridine	0.732	0.830	0.000	0.400	3.783	0.7977	-46.20	24
Quinoline	1.268	0.970	0.000	0.540	5.457	1.0440	-58.20	25
Methanethiol	0.400	0.600	0.000	0.120	1.640	0.4130	-25.80	22,25
Ethanethiol	0.392	0.350	0.000	0.240	2.173	0.5539	-28.30	25
1-Propanethiol	0.385	0.350	0.000	0.240	2.685	0.6948	-30.20	28
1-Butanethiol	0.382	0.350	0.000	0.240	3.243	0.8357	-36.29	28
Dimethylsulfide	0.404	0.430	0.000	0.270	2.037	0.5539	-31.50	28
Diethylsulfide	0.373	0.380	0.000	0.330	3.021	0.8357	-40.20	28
Dipropyl sulfide	0.358	0.380	0.000	0.340	4.010	1.1175	-47.60	28
Thiophene	0.687	0.560	0.000	0.150	2.819	0.6410	-29.90	22
Acetic acid	0.265	0.650	0.610	0.440	1.750	0.4648	-52.80	44
Propanoic acid	0.233	0.650	0.610	0.440	2.276	0.6057	-56.50	44
Butanoic acid	0.210	0.640	0.610	0.450	2.750	0.7466	-59.50	24
2-Methoxyphenol	0.837	0.910	0.220	0.520	4.449	0.9750	-62.60	25
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-0.67	22
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-3.90	22
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-12.20	22
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-15.60	22
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	-19.40	22
Radon	0.000	0.000	0.000	0.000	0.877	0.3840	-24.00	22
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-0.402	43
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-1.205	43
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-1.042	43
Nitrous Oxide	0.068	0.350	0.000	0.100	0.164	0.2810	-19.80	44
Nitric Oxide	0.370	0.020	0.000	0.090	-0.590	0.2026	-11.90	44
Carbon Monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-11.13	22
Carbon Dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	-17.90	25
Benzyl alcohol	0.803	0.870	0.330	0.560	4.221	0.9160	-66.94	22
2-Chlorobiphenyl	1.480	1.070	0.000	0.200	6.336	1.4466	-42.80	25
2,3-Dichlorobiphenyl	1.630	1.200	0.000	0.180	7.168	1.5690	-45.60	25
2,4-Dichlorobiphenyl	1.620	1.200	0.000	0.180	7.042	1.5690	-43.00	25

2,4'-Dichlorobiphenyl	1.620	1.200	0.000	0.180	7.197	1.5690	-44.20	25
2,5-Dichlorobiphenyl	1.630	1.200	0.000	0.180	7.001	1.5690	-45.60	25
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896	-5.93	24
Isophorone	0.511	1.120	0.000	0.530	4.740	1.2408	-59.10	25
Morpholine	0.434	0.790	0.060	0.910	3.289	0.7221	-69.50	24
N-Methylmorpholine	0.333	0.740	0.000	0.900	3.270	0.8630	-68.70	24
Propanamide	0.440	1.300	0.550	0.660	3.510	0.6468	-73.40	44
N,N-Dimethylformamide	0.367	1.310	0.000	0.740	3.173	0.6468	-62.90	24
Dimethyl sulfoxide	0.522	1.720	0.000	0.970	3.459	0.6126	-71.90	24
N-Methylpyrrolidine	0.300	0.980	0.000	0.400	3.132	0.8043	-63.40 *	24
Hexan-3-one	0.136	0.660	0.000	0.510	3.310	0.9697	-46.00	25
2-Nonanone	0.119	0.680	0.000	0.510	4.735	1.3924	-65.30	25
cis 1,2-Cyclohexanediol	0.600	0.860	0.500	0.860	4.203	0.9628	-82.40	68
12-Crown-4	0.420	0.990	0.000	1.390	5.135	1.3620	-94.65	67
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	-119.28	67
18-Crown-6	0.400	1.340	0.000	2.130	7.919	2.0430	-149.51	67
Erithritol	0.620	1.600	0.480	1.390		0.9070	-114.00	69

* Not included in the regression analyses.

Table S2. Values of the gas to 1-octanol solvation enthalpy in kJ/mol at 298K for 138 solutes, together with the solute descriptors.

Solute	E	S	A	B	L	V	Exp Value	Ref
Sulphur hexafluoride	-0.600	-0.200	0.00	0.00	-0.120	0.4643	-6.56	22
Methane	0.000	0.000	0.00	0.00	-0.323	0.2495	-3.90	22
Pentane	0.000	0.000	0.00	0.00	2.162	0.8131	-25.52	42
Hexane	0.000	0.000	0.00	0.00	2.668	0.9540	-30.33	42
Heptane	0.000	0.000	0.00	0.00	3.173	1.0949	-35.31	42
3-Ethylpentane	0.000	0.000	0.00	0.00	3.091	1.0949	-34.23	31
Octane	0.000	0.000	0.00	0.00	3.677	1.2358	-40.08	42
Nonane	0.000	0.000	0.00	0.00	4.182	1.3767	-44.89	42
Decane	0.000	0.000	0.00	0.00	4.686	1.5176	-49.71	42
Dodecane	0.000	0.000	0.00	0.00	5.696	1.7994	-59.12	42
Hexadecane	0.000	0.000	0.00	0.00	7.714	2.3630	-78.20	42
Cyclohexane	0.305	0.100	0.00	0.00	2.964	0.8454	-35.50	33
Methylcyclohexane	0.244	0.060	0.00	0.00	3.319	0.9863	-34.33	31
Ethene	0.107	0.100	0.00	0.07	0.289	0.3474	-6.25	62
1-Pentene	0.093	0.080	0.00	0.07	2.047	0.7701	-22.40	64
1-Hexene	0.078	0.080	0.00	0.07	2.572	0.9110	-26.56	64
Cyclohexene	0.395	0.200	0.00	0.10	3.021	0.8025	-38.14	64
Tetrafluoromethane	-0.580	-0.260	0.00	0.00	-0.817	0.3202	0.92	22
Dichloromethane	0.387	0.570	0.10	0.05	2.019	0.4943	-27.86	49
Trichloromethane	0.425	0.490	0.15	0.02	2.480	0.6167	-32.69	49
Tetrachloromethane	0.458	0.380	0.00	0.00	2.823	0.7391	-28.76	49
1,1-Dichloroethane	0.322	0.490	0.10	0.10	2.316	0.6352	-28.68	49
1,2-Dichloroethane	0.416	0.640	0.10	0.11	2.573	0.6352	-29.58	49
1,1,1-Trichloroethane	0.369	0.410	0.00	0.09	2.733	0.7576	-26.45	49
1,1,2-Trichloroethane	0.499	0.680	0.13	0.13	3.290	0.7576	-36.73	49
1,1,1,2-Tetrachloroethane	0.542	0.630	0.10	0.08	3.641	0.8800	-42.27	49
1-Chloropropane	0.216	0.400	0.00	0.10	2.202	0.6537	-26.02	31
1,2-Dichloropropane	0.369	0.630	0.00	0.17	2.836	0.7761	-32.69	49
1-Chlorobutane	0.210	0.400	0.00	0.10	2.722	0.7946	-31.00	31
2-Chlorobutane	0.189	0.350	0.00	0.12	2.540	0.7955	-28.87	31
1-Chloropentane	0.208	0.380	0.00	0.09	3.223	0.9355	-35.92	31
1-Chlorohexane	0.201	0.400	0.00	0.10	3.777	1.0770	-40.43	31
1-Chlorooctane	0.191	0.400	0.00	0.09	4.708	1.3585	-49.97	31
Dibromomethane	0.714	0.690	0.11	0.07	2.886	0.5995	-38.08	49
Trichloroethylene	0.524	0.370	0.08	0.03	2.997	0.7146	-34.43	65
Diethyl ether	0.041	0.250	0.00	0.45	2.015	0.7309	-24.86	33
Di-n-propyl ether	0.008	0.250	0.00	0.45	2.954	1.0127	-33.19	33
Di-isopropyl ether	-0.060	0.160	0.00	0.58	2.530	1.0127	-31.04	31
Dibutyl ether	0.000	0.250	0.00	0.45	3.924	1.2950	-42.58	33
Methyl tert-butyl ether	0.024	0.210	0.00	0.59	2.380	0.8718	-28.03	33

Tetrahydrofuran	0.289	0.520	0.00	0.48	2.636	0.6223	-28.32	33
Tetrahydropyran	0.275	0.470	0.00	0.55	3.057	0.7672	-30.66	33
1,4-Dioxane	0.329	0.750	0.00	0.64	2.892	0.6810	-28.73	48
Propanone	0.179	0.700	0.04	0.49	1.696	0.5470	-22.37	33
Butanone	0.166	0.700	0.00	0.51	2.287	0.6879	-27.36	33
Pentan-2-one	0.143	0.680	0.00	0.51	2.755	0.8288	-31.03	33
Pentan-3-one	0.154	0.660	0.00	0.51	2.811	0.8288	-32.86	33
Hexan-2-one	0.136	0.680	0.00	0.51	3.286	0.9697	-36.12	33
Heptan-4-one	0.110	0.660	0.00	0.51	3.705	1.1106	-40.47	33
Nona-2-one	0.119	0.680	0.00	0.51	4.731	1.3924	-50.29	31
Nonan-5-one	0.103	0.660	0.00	0.51	4.698	1.3924	-47.19	31
Cyclopentanone	0.373	0.860	0.00	0.52	3.221	0.7200	-34.34	33
Cyclohexanone	0.403	0.860	0.00	0.56	3.792	0.8610	-37.27	31
Acetophenone	0.818	1.010	0.00	0.48	4.501	1.0140	-50.23	31
Methyl acetate	0.142	0.640	0.00	0.45	1.911	0.6057	-24.62	31
Ethyl acetate	0.106	0.620	0.00	0.45	2.314	0.7466	-27.78	31
Propyl acetate	0.092	0.600	0.00	0.45	2.819	0.8875	-33.00	31
Butyl acetate	0.071	0.600	0.00	0.45	3.353	1.0284	-37.13	31
Pentyl acetate	0.067	0.600	0.00	0.45	3.844	1.1693	-41.31	31
Methyl formate	0.192	0.680	0.00	0.38	1.285	0.4648	-21.40	31
Propyl formate	0.132	0.630	0.00	0.38	2.433	0.7466	-30.39	31
Methyl propionate	0.128	0.600	0.00	0.45	2.431	0.7466	-26.67	31
Ethyl propionate	0.087	0.580	0.00	0.45	2.807	0.8875	-32.54	31
Methyl butanoate	0.106	0.600	0.00	0.45	2.943	0.8875	-33.04	31
Methyl pentanoate	0.108	0.600	0.00	0.45	3.442	1.0284	-37.02	31
Ethyl benzoate	0.689	0.850	0.00	0.46	5.075	1.2140	-54.52	31
Methanol	0.278	0.440	0.43	0.47	0.970	0.3082	-37.08	31
Ethanol	0.246	0.420	0.37	0.48	1.485	0.4491	-41.79	31
Propan-1-ol	0.236	0.420	0.37	0.48	2.031	0.5900	-46.96	31
Butan-1-ol	0.224	0.420	0.37	0.48	2.601	0.7309	-51.84	33
2-Butanol	0.217	0.360	0.33	0.56	2.338	0.7309	-49.40	33
tert-Butanol	0.180	0.300	0.31	0.60	1.963	0.7309	-46.99	33
Pentan-1-ol	0.219	0.420	0.37	0.48	3.106	0.8718	-56.74	31
2,2-Dimethyl-1-propanol	0.220	0.360	0.37	0.53	2.650	0.8718	-53.64	31
Hexan-1-ol	0.210	0.420	0.37	0.48	3.610	1.0170	-61.49	31
Octan-1-ol	0.199	0.420	0.37	0.48	4.619	1.2950	-70.98	31
Decan-1-ol	0.191	0.420	0.37	0.48	5.628	1.5763	-81.40	31
Benzene	0.610	0.520	0.00	0.14	2.786	0.7176	-30.98	31
Toluene	0.601	0.520	0.00	0.14	3.325	0.8573	-35.99	31
Ethylbenzene	0.613	0.510	0.00	0.15	3.778	0.9982	-39.91	31
o-Xylene	0.663	0.560	0.00	0.16	3.939	0.9982	-41.53	31
m-Xylene	0.623	0.520	0.00	0.16	3.839	0.9982	-41.00	31
p-Xylene	0.613	0.520	0.00	0.16	3.839	0.9982	-40.59	31
1,3,5-Trimethylbenzene	0.649	0.520	0.00	0.19	4.344	1.1391	-45.88	31
1,2-Dichlorobenzene	0.872	0.780	0.00	0.04	4.518	0.9612	-49.30	63
1,2,3-Trichlorobenzene	1.030	0.860	0.00	0.00	5.419	1.0836	-55.70	63

1,2,3,4-Tetrachlorobenzene	1.180	0.920	0.00	0.00	6.171	1.2060	-62.30	63
1,2,4,5-Tetrachlorobenzene	1.160	0.860	0.00	0.00	5.926	1.2060	-60.80	63
Hexachlorobenzene	1.490	0.990	0.00	0.00	7.624	1.4508	-75.20	63
Aniline	0.955	0.960	0.26	0.41	3.934	0.8162	-51.19	31
Nitrobenzene	0.871	1.110	0.00	0.28	4.557	0.8906	-47.14	31
Phenanthrene	2.060	1.290	0.00	0.29	7.632	1.4544	-75.50	50
Pyrene	2.808	1.710	0.00	0.28	8.833	1.5846	-76.30	50
Butyronitrile	0.180	0.900	0.00	0.36	2.548	0.6860	-31.39	50
Propylamine	0.225	0.350	0.16	0.61	2.141	0.6311	-40.90	33
Butylamine	0.224	0.350	0.16	0.61	2.618	0.7720	-45.11	33
Pentylamine	0.211	0.350	0.16	0.61	3.139	0.9129	-50.03	33
Diethylamine	0.154	0.300	0.08	0.69	2.395	0.7720	-42.52	33
Dipropylamine	0.124	0.300	0.08	0.69	3.351	1.0538	-50.82	33
Dibutylamine	0.107	0.300	0.08	0.69	4.349	1.3356	-60.07	33
Triethylamine	0.101	0.150	0.00	0.79	3.040	1.0538	-43.58	33
Piperidine	0.422	0.460	0.10	0.69	3.304	0.8043	-48.99	33
N-Methylpiperidine	0.318	0.340	0.00	0.72	3.330	0.9452	-43.24	33
Helium	0.000	0.000	0.00	0.00	-1.741	0.0680	3.93	22
Argon	0.000	0.000	0.00	0.00	-0.688	0.1900	-0.67	22
Xenon	0.000	0.000	0.00	0.00	0.378	0.3290	-9.64	47
Oxygen	0.000	0.000	0.00	0.00	-0.723	0.1830	-1.17	22
Nitrogen	0.000	0.000	0.00	0.00	-0.978	0.2222	2.51	22
Carbon Monoxide	0.000	0.000	0.00	0.04	-0.836	0.2220	0.21	22
Carbon Dioxide	0.000	0.280	0.05	0.10	0.058	0.2809	-9.13	51
3-Chlorobiphenyl	1.510	1.050	0.000	0.180	6.667	1.4466	-66.44	52
2,2',4,5'-Tetrachlorobiphenyl	1.890	1.480	0.000	0.150	8.186	1.8138	-76.23	52
2,2',5,6'-Tetrachlorobiphenyl	1.870	1.480	0.000	0.150	7.949	1.8138	-75.92	52
2,3,3',4,4'-Pentachlorobiphenyl	2.040	1.590	0.000	0.110	9.594	1.0362	-89.57	52
2,3',4,4',5-Pentachlorobiphenyl	2.060	1.590	0.000	0.110	9.396	1.0362	-89.86	52
3,3',4,4',5-Pentachlorobiphenyl	2.110	1.570	0.000	0.090	9.884	1.0362	-93.25	52
2,2',3,4,4',5'-Hexachlorobiphenyl	2.180	1.740	0.000	0.110	9.772	2.0586	-89.90	52
2,2',4,4',5,5'-Hexachlorobiphenyl	2.180	1.740	0.000	0.110	9.587	2.0586	-87.77	52
2,2',3,3',4,4',6-Heptachlorobiphenyl	2.300	1.870	0.000	0.090	10.031	2.1810	-91.08	52
2,2',3,4,4',5,6-Heptachlorobiphenyl	2.300	1.870	0.000	0.090	9.965	2.1810	-86.83	52
1,4-Dichloronaphthalene	1.570	1.060	0.000	0.090	6.757	1.3302	-62.19	50
1,3,5-Trichloronaphthalene	1.690	1.120	0.000	0.000	7.585	1.4526	-72.49	50
1,4,5-Trichloronaphthalene	1.690	1.120	0.000	0.000	8.070	1.4526	-74.60	50
1,2,4,5-Tetrachloronaphthalene	1.810	1.240	0.000	0.000	8.674	1.5750	-81.62	50
1,2,4,8-Tetrachloronaphthalene	1.810	1.240	0.000	0.000	8.736	1.5750	-80.53	50
1,2,5,8-Tetrachloronaphthalene	1.810	1.240	0.000	0.000	8.819	1.5750	-80.05	50
1,4,5,8-Tetrachloronaphthalene	1.810	1.180	0.000	0.000	9.135	1.5750	-80.53	50
1,2,4,5,7-Pentachloronaphthalene	1.930	1.300	0.000	0.000	9.225	1.6974	-84.32	50
1,2,4,6,8-Pentachloronaphthalene	1.930	1.300	0.000	0.000	9.280	1.6974	-84.57	50
1,2,3,4,6-Pentachloronaphthalene	1.930	1.360	0.000	0.000	9.196	1.6974	-88.63	50

1,2,4,7,8-Pentachloronaphthalene	1.930	1.360	0.000	0.000	9.462	1.6974	-85.24	50
1,2,3,5,8-Pentachloronaphthalene	1.930	1.360	0.000	0.000	9.496	1.6974	-89.69	50
1,2,4,5,8-Pentachloronaphthalene	1.930	1.360	0.000	0.000	9.594	1.6974	-92.12	50
1,2,3,5,7,8-Hexachloronaphthalene	2.050	1.420	0.000	0.000	10.242	1.8198	-93.99	50
1,2,3,4,5,6-Hexachloronaphthalene	2.050	1.420	0.000	0.000	10.537	1.8198	-89.34	50
1,2,3,4,5,8-Hexachloronaphthalene	2.050	1.420	0.000	0.000	10.657	1.8198	-96.50	50
N-Methylpyrrolidine	0.303	0.500	0.000	0.710	2.808	0.8043	-40.33	33
Pyrrolidine	0.406	0.670	0.120	0.630	2.893	0.6634	-47.85	33

TABLE 3. CAS Registry Numbers for Solutes Considered in the Present Study

Solute	CAS Registry Numbers
Chlorine gas	7782-50-5
Hydrogen sulfide	7783-06-4
Hydrogen selenide	7783-07-5
Chlorine dioxide	10049-04-4
Sulphur hexafluoride	2551-62-4
Ammonia	7664-41-7
Methane	74-82-8
Ethane	74-84-0
Propane	74-98-6
Butane	106-97-8
2-Methylpropane	75-28-5
Pentane	109-66-0
2,2-Dimethylpropane	463-82-1
Hexane	110-54-3
2-Methylpentane	107-83-5
3-Methylpentane	96-14-0
2,3-Dimethylbutane	79-29-8
Heptane	142-82-5
Octane	111-65-9
2,2,4-Trimethylpentane	540-84-1
2,3,4-Trimethylpentane	565-75-3
Nonane	111-84-2
Decane	124-18-5
Dodecane	112-40-3
Hexadecane	544-76-4
Cyclopropane	75-19-4
Cyclopentane	287-92-3
Cyclohexane	110-82-7
Methylcyclohexane	108-87-2
cis-1,2-Dimethylcyclohexane	1678-91-7
trans-1,2-Dimethylcyclohexane	6876-23-9
Ethylcyclohexane	1678-91-7
Cyclooctane	292-64-8
Ethene	74-85-1

Propene	115-07-1
1-Butene	106-98-9
1-Pentene	109-67-1
1-Hexene	592-41-6
1-Octene	111-66-0
2-Methylpropene	115-11-7
2-Methyl-2-butene	513-35-9
1,3-Butadiene	106-99-0
Cyclohexene	110-83-8
Cyclooctene	931-88-4
Propyne	74-99-7
1-Butyne	107-00-6
Fluoromethane	593-53-3
Difluoromethane	75-10-5
Tetrafluoromethane	75-73-0
1,1-Difluoroethane	75-37-6
Trifluoromethane	75-46-7
1,1,1,2-Tetrafluoroethane	359-35-3
Pentafluoroethane	354-33-6
1,1,1,2,3,3,3-Heptafluoropropane	431-89-0
Chloromethane	74-87-3
Dichloromethane	75-09-2
Trichloromethane	67-66-3
Tetrachloromethane	56-23-5
Chloroethane	75-00-3
1,1-Dichloroethane	75-34-3
1,2-Dichloroethane	107-06-2
1,1,1-Trichloroethane	71-55-6
1,1,2-Trichloroethane	79-00-5
1,1,2,2-Tetrachloroethane	79-34-5
1,1,1,2-Tetrachloroethane	630-20-6
1-Chloropropane	540-54-5
1,2-Dichloropropane	78-87-5
1,3-Dichloropropane	142-28-9
1-Chlorobutane	109-69-3
2-Chlorobutane	78-86-4
1-Chloropentane	543-59-9
1-Chlorohexane	544-10-5

1-Chlorooctane	111-85-3
Tetrafluoroethene	116-14-3
Hexafluoropropene	116-15-4
1,1-Dichloroethylene	75-35-4
cis-1,2-Dichloroethylene	156-59-2
trans-1,2-Dichloroethylene	156-60-5
Trichloroethylene	79-01-6
Tetrachloroethane	127-18-4
Bromomethane	74-83-9
Dibromomethane	74-95-3
Tribromomethane	75-25-2
Bromoethane	74-96-4
2-Methyl-2-bromopropane	507-19-7
Iodomethane	74-88-4
Diiodomethane	75-11-6
Iodoethane	75-03-6
1-Iodopropane	107-08-4
2-Iodopropane	75-30-9
Fluorochloromethane	593-70-4
Difluorochloromethane	75-45-6
Bromodichloromethane	75-27-4
Chlorodibromomethane	124-48-1
Fluorotrichloromethane	75-69-4
Difluorodichloromethane	75-71-8
1,1,2-Trichlorotrifluoroethane	76-13-1
1,2-Dichlorotetrafluoroethane	76-14-2
Dimethyl ether	115-10-6
Diethyl ether	60-29-7
Di-n-propyl ether	111-43-3
Di-isopropyl ether	108-20-3
Dibutyl ether	142-96-1
Methyl propyl ether	557-17-5
Ethyl butyl ether	628-81-9
Methyl tert-butyl ether	1634-04-4
Ethyl tert-butyl ether	637-92-3
Methyl tert-pentyl ether	994-05-8
Tetrahydrofuran	109-99-9
2,5-Dimethyltetrahydrofuran	1003-38-9

2-Methyltetrahydrofuran	96-47-9
Tetrahydropyran	142-68-7
1,4-Dioxane	123-91-1
1,2-Dimethoxyethane	110-71-4
1,2-Diethoxyethane	629-14-1
1-Methoxy-2-ethoxyethane	5137-45-1
1-Methoxy-2-propoxyethane	17081-22-0
1,2-Dipropoxyethane	18854-56-3
3,6,9-Trioxoundecane	111-96-6
2,5,8,11-Tetraoxododecane	112-49-2
2,5,8,11,14-Pentaoxopentadecane	143-24-8
12-Crown-4	294-93-9
15-Crown-5	33100-27-5
18-Crown-6	17455-13-9
Methoxyflurane	76-38-0
Isoflurane	26675-46-7
Propanone	67-64-1
Butanone	78-93-3
Pentan-2-one	107-87-9
Pentan-3-one	96-22-0
Hexan-2-one	591-78-6
Hexan-3-one	589-38-8
4-Methylpentan-2-one	108-10-1
Methyl isopropyl ketone	563-80-4
3,3-Dimethyl-2-butanone	75-97-8
Diisopropyl ketone (2,4-Dimethyl-3-pentanone)	565-84-0
Heptan-2-one	110-43-0
Heptan-4-one	123-19-3
Octan-2-one	111-13-7
Nonan-2-one	821-55-6
Nonan-5-one	502-56-7
Cyclopentanone	120-92-3
Cyclohexanone	108-94-1
Acetophenone	98-86-2
Propiophenone	93-55-0
Methyl acetate	79-20-9
Ethyl acetate	141-78-6
Propyl acetate	109-60-4

Isopropyl acetate	108-21-4
Butyl acetate	123-86-4
Isobutyl acetate	110-19-0
sec-Butyl acetate	105-46-4
tert-Butyl acetate	540-88-5
Pentyl acetate	628-63-7
Isopentyl acetate	123-92-2
Hexyl acetate	142-92-7
Methyl formate	107-31-3
Ethyl formate	109-94-4
Propyl formate	110-74-7
Isopropyl formate	625-55-8
Isobutyl formate	542-55-2
Pentyl formate	638-49-3
3-Methylbutyl formate	110-45-2
Methyl propanoate	554-12-1
Ethyl propanoate	105-37-3
Propyl propanoate	106-36-5
Butyl propanoate	590-01-2
Isobutyl propanoate	540-42-1
Methyl butanoate	623-42-7
Ethyl butanoate	105-54-5
Propyl butanoate	105-66-8
Butyl butanoate	109-21-7
Methyl 2-methylpropanoate	547-63-7
Ethyl 2-methylpropanoate	97-62-1
Isobutyl 2-methylpropanoate	97-85-8
Methyl pentanoate	624-24-8
Ethyl pentanoate	539-82-2
Methyl 2,2-dimethylpropanoate	598-98-1
Ethyl 2,2-dimethylpropanoate	3938-95-2
Ethyl 3-methylbutanoate	108-64-5
Ethyl 2-methylbutanoate	7452-79-1
Methyl hexanoate	106-70-7
Ethyl hexanoate	123-66-0
Methyl benzoate	93-58-3
Ethyl benzoate	93-89-0
Nitromethane	75-52-5

Nitroethane	79-24-3
1-Nitropropane	108-03-2
2-Nitropropane	79-46-9
Methanol	67-56-1
Ethanol	64-17-5
Propan-1-ol	71-23-8
Propan-2-ol	67-63-0
Butan-1-ol	71-36-3
2-Butanol	78-92-2
2-Methylpropan-1-ol	78-83-1
tert-Butanol	75-65-0
Pentan-1-ol	71-41-0
3-Methyl-1-butanol	123-51-3
2-Pentanol	6032-29-7
3-Pentanol	584-02-1
Hexan-1-ol	111-27-3
Hexan-3-ol	623-37-0
2-Methyl-2-butanol	75-85-4
4-Methyl-2-pentanol	108-11-2
Heptan-1-ol	111-70-6
Heptane-2-ol	543-49-7
Heptan-4-ol	589-55-9
Octan-1-ol	111-87-5
Decan-1-ol	112-30-1
Dodecan-1-ol	112-53-8
Cyclopentanol	96-41-3
Cyclohexanol	108-93-0
Cycloheptanol	502-41-0
Ethan-1,2-diol	107-21-1
Propan-1,3-diol	504-63-2
Butan-1,4-diol	110-63-4
Glycerol	56-81-5
2-Methoxyethanol	109-86-4
2-Ethoxyethanol	110-80-5
2-Propoxyethanol	2807-30-9
2-Butoxyethanol	111-76-2
Benzene	71-43-2
Toluene	108-88-3

Ethylbenzene	100-41-4
o-Xylene	95-47-6
m-Xylene	108-38-3
p-Xylene	106-42-3
Propylbenzene	103-65-1
Isopropylbenzene	98-82-8
1,2,3-Trimethylbenzene	526-73-8
1,2,4-Trimethylbenzene	95-63-6
1,3,5-Trimethylbenzene	108-67-8
4-Isopropyltoluene	99-87-6
Butylbenzene	104-51-8
Pentylbenzene	538-68-1
Hexylbenzene	1077-16-3
1,4-Diethylbenzene	105-05-5
Styrene	100-42-5
Fluorobenzene	462-06-6
Chlorobenzene	108-90-7
1,2-Dichlorobenzene	95-50-1
1,3-Dichlorobenzene	541-73-1
1,4-Dichlorobenzene	106-46-7
1,2,3-Trichlorobenzene	87-61-6
1,3,5-Trichlorobenzene	108-70-3
1,2,3,4-Tetrachlorobenzene	634-66-2
Pentachlorobenzene	608-93-5
Hexachlorobenzene	118-74-1
2-Chlorotoluene	95-49-8
3-Chlorotoluene	108-41-8
4-Chlorotoluene	106-43-4
Bromobenzene	108-86-1
Phenyl methyl ether	1100-66-3
Aniline	62-53-3
2-Ethylaniline	578-54-1
4-Ethylaniline	589-16-2
2,4-Dimethylaniline	95-68-1
2,5-Dimethylaniline	95-78-3
2,6-Dimethylaniline	87-62-7
N,N-Dimethylaniline	121-69-7
N,N-Diethylaniline	91-66-7

Nitrobenzene	98-95-3
2-Nitrotoluene	88-72-2
3-Nitrotoluene	99-08-1
Phenol	108-95-2
2-Methylphenol	95-48-7
3-Methylphenol	108-39-4
4-Methylphenol	106-44-5
4-tert-Butylphenol	98-54-4
3-Chlorophenol	108-43-0
4-Chlorophenol	106-48-9
3-Cyanophenol	873-62-1
4-Cyanophenol	767-00-0
2-Nitrophenol	88-75-5
3-Nitrophenol	554-84-7
4-Nitrophenol	100-02-7
Biphenyl	92-52-4
Naphthalene (approx)	91-20-3
1-Methylnaphthalene	90-12-0
2-Methylnaphthalene	91-57-6
Acenaphthene	83-32-9
Fluorene	86-73-7
Propanal	123-38-6
Pentanal	110-62-3
Hexanal	66-25-1
Heptanal	111-71-7
Octanal	124-13-0
Isobutyl aldehyde	78-84-2
Benzaldehyde	100-52-7
3-Hydroxybenzaldehyde	100-83-4
Acetonitrile	75-05-8
Propionitrile	107-12-0
Butyronitrile	109-74-0
Pentanenitrile	110-59-8
2-Cyanopropane	78-82-0
1,2-Dicyanoethane	110-61-2
1,3-Dicyanopropane	544-13-8
1,4-Dicyanobutane	111-69-3
Benzonitrile	100-47-0

2,2,2-Trifluoroethanol	75-89-8
1,1,1-Trifluoropropan-2-ol	374-01-6
2,2,3,3-Tetrafluoropropan-1-ol	76-37-9
2,2,3,3,3-Pentafluoropropan-1-ol	422-05-9
1,1,1,3,3,3-Hexafluoropropan-2-ol	920-66-1
Methylamine	74-89-5
Ethylamine	75-04-7
Propylamine	107-104
Isopropylamine	75-31-0
Butylamine	109-73-9
sec-Butylamine	13952-84-6
tert-Butylamine	75-64-9
Pentylamine	110-58-7
Hexylamine	111-26-2
Octylamine	111-86-4
Dimethylamine	124-40-3
Diethylamine	109-89-7
Dipropylamine	142-84-7
Dibutylamine	111-92-2
Trimethylamine	75-50-3
Triethylamine	121-44-8
1,2-Diaminoethane	107-15-3
1,3-Diaminopropane	109-76-2
1,4-Diaminobutane	110-60-1
1,5-Diaminopentane	462-94-2
Piperidine	110-89-4
N-Methylpiperidine	626-67-5
pyridine	110-86-1
2-Methylpyridine	109-06-8
3-Methylpyridine	108-99-6
4-Methylpyridine	108-89-4
3-Ethylpyridine	536-78-7
4-Ethylpyridine	536-75-4
2,3-Dimethylpyridine	583-61-9
2,4-Dimethylpyridine	108-47-4
2,5-Dimethylpyridine	589-93-5
2,6-Dimethylpyridine	108-48-5
3,4-Dimethylpyridine	583-58-4

3,5-Dimethylpyridine	591-22-0
2-Chloropyridine	109-09-1
3-Chloropyridine	626-60-8
Quinoline	91-22-5
Methanethiol	74-93-1
Ethanethiol	75-08-1
1-Propanethiol	107-03-9
1-Butanethiol	109-79-5
Dimethylsulfide	75-18-3
Diethylsulfide	352-93-2
Dipropyl sulfide	111-47-7
Thiophene	110-02-1
Acetic acid	64-19-7
Propanoic acid	79-09-4
Butanoic acid	107-92-6
2-Methoxyphenol	90-05-1
Helium	7440-59-7
Neon	7440-01-9
Argon	7440-37-1
Krypton	7439-90-9
Xenon	7440-63-3
Radon	10043-92-2
Hydrogen	1333-74-0
Oxygen	7782-44-7
Nitrogen	7727-37-9
Nitrous Oxide	10102-43-9
Nitric Oxide	102-43-9
Carbon Monoxide	630-08-0
Carbon Dioxide	124-38-9
Benzyl alcohol	100-51-6
2-Chlorobiphenyl	2051-60-7
3-Chlorobiphenyl	2051-61-6
2,3-Dichlorobiphenyl	16605-91-7
2,4-Dichlorobiphenyl	33284-50-3
2,4'-Dichlorobiphenyl	34883-43-7
2,5-Dichlorobiphenyl	34883-39-1
2,2',4,5'-Tetrachlorobiphenyl	41464-40-8
2,2',5,6'-Tetrachlorobiphenyl	41464-41-9

2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4
2,3',4,4',5-Pentachlorobiphenyl	31508-00-6
3,3',4,4',5-Pentachlorobiphenyl	57465-28-8
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-27-1
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1
2,2',3,3',4,4',6-Heptachlorobiphenyl	52663-71-5
2,2',3,4,4',5,6-Heptachlorobiphenyl	74472-47-2
1,4-Dichloronaphthalene	1825-31-6
1,3,5-Trichloronaphthalene	51570-43-5
1,4,5-Trichloronaphthalene	2437-55-0
1,2,4,5-Tetrachloronaphthalene	5733-54-6
1,2,4,8-Tetrachloronaphthalene	6529-87-9
1,2,5,8-Tetrachloronaphthalene	149864-80-2
1,4,5,8-Tetrachloronaphthalene	3432-57-3
1,2,4,5,7-Pentachloronaphthalene	150224-19-4
1,2,4,6,8-Pentachloronaphthalene	150224-22-9
1,2,3,4,6-Pentachloronaphthalene	67922-26-3
1,2,4,7,8-Pentachloronaphthalene	150224-21-8
1,2,3,5,8-Pentachloronaphthalene	150224-24-1
1,2,4,5,8-Pentachloronaphthalene	150224-25-2
1,2,3,5,7,8-Hexachloronaphthalene	103426-94-4
1,2,3,4,5,6-Hexachloronaphthalene	58877-88-6
1,2,3,4,5,8-Hexachloronaphthalene	103426-93-3
Isophorone	78-59-1
Morpholine	110-91-8
N-Methylmorpholine	109-02-4
Propanamide	79-05-0
N,N-Dimethylformamide	68-12-2
Dimethyl sulfoxide	67-68-5
cis 1,2-Cyclohexanediol	1792-81-0
Erythritol	149-32-6

Table S4. First Training and Test Set Analyses for Water Data Set

Training Set 1	Test Set 1
Chlorine gas	Hydrogen selenide
Hydrogen sulfide	Ammonia
Chlorine dioxide	2,2-Dimethylpropane
Sulphur hexafluoride	2-Methylpentane
Methane	3-Methylpentane
Ethane	2,3-Dimethylbutane
Propane	Octane
Butane	Cyclopropane
2-Methylpropane	cis-1,2-Dimethylcyclohexane
Pentane	trans-1,2-Dimethylcyclohexane
Hexane	Propene
Heptane	2-Methyl-2-butene
2,2,4-Trimethylpentane	1,3-Butadiene
2,3,4-Trimethylpentane	Cyclohexene
Cyclopentane	Propyne
Cyclohexane	1-Butyne
Ethylcyclohexane	Difluoromethane
Cyclooctane	1,1-Difluoroethane
Ethene	Trifluoromethane
1-Butene	1,1,1,2-Tetrafluoroethane
1-Hexene	1,1,1,2,3,3,3-Heptafluoropropane
1-Octene	Chloromethane
2-Methylpropene	Trichloromethane
Cyclooctene	Tetrachloromethane
Fluoromethane	1,1-Dichloroethane
Tetrafluoromethane	1,2-Dichloroethane
Pentafluoroethane	1,1,2,2-Tetrachloroethane
Dichloromethane	1,3-Dichloropropane
Chloroethane	1-Chlorobutane
1,1,1-Trichloroethane	2-Chlorobutane
1,1,2-Trichloroethane	trans-1,2-Dichloroethylene
1,1,1,2-Tetrachloroethane	Tribromomethane
1-Chloropropane	Bromoethane
1,2-Dichloropropane	2-Methyl-2-bromopropane
1-Chloropentane	Iodomethane
1-Chlorohexane	2-Iodopropane
Tetrafluoroethene	Fluorochloromethane
Hexafluoropropene	Chlorodibromomethane
1,1-Dichloroethylene	Fluorotrichloromethane
cis-1,2-Dichloroethylene	1,1,2-Trichlorotrifluoroethane
Trichloroethylene	Dimethyl ether
Bromomethane	Diethyl ether
Dibromomethane	Di-isopropyl ether
Diiodomethane	Dibutyl ether
Iodoethane	Methyl propyl ether
1-Iodopropane	Ethyl tert-butyl ether

Difluorochloromethane
Bromodichloromethane
Difluorodichloromethane
1,2-Dichlorotetrafluoroethane
Di-n-propyl ether
Ethyl butyl ether
Methyl tert-butyl ether
Tetrahydrofuran
2,5-Dimethyltetrahydrofuran
2-Methyltetrahydrofuran
1,4-Dioxane
15-Crown-5
18-Crown-6
Methoxyflurane
Isoflurane
Hexan-2-one
Hexan-3-one

Methyl isopropyl ketone
Octan-2-one
Nonan-2-one
Cyclohexanone
Methyl acetate
Propyl acetate
Isopropyl acetate
tert-Butyl acetate
Pentyl acetate
Ethyl formate
Isopropyl formate
Isobutyl formate
Pentyl formate
3-Methylbutyl formate
Methyl propanoate
Butyl propanoate
Methyl butanoate
Ethyl butanoate
Methyl 2-methylpropanoate
Methyl pentanoate
Ethyl pentanoate
Ethyl 2,2-dimethylpropanoate
Ethyl 2-methylbutanoate
Methyl hexanoate
Ethyl hexanoate
Nitroethane
1-Nitropropane
2-Nitropropane
Methanol
Ethanol
Propan-1-ol

Methyl tert-pentyl ether
Tetrahydropyran
1,2-Dimethoxyethane
1,2-Diethoxyethane
1-methoxy-2-ethoxyethane
1-methoxy-2-propoxyethane
1,2-dipropoxyethane
3,6,9-trioxoundecane
2,5,8,11-tetraoxododecane
2,5,8,11,14-pentaoxopentadecane
12-Crown-4
Propanone
Butanone
Pentan-2-one
Pentan-3-one
4-Methylpentan-2-one
3,3-Dimethyl-2-butanone
Diisopropyl ketone (2,4-Dimethyl-3-pentanone)
Heptan-2-one
Heptan-4-one
Nonan-5-one
Cyclopentanone
Acetophenone
Propiophenone
Ethyl acetate
Butyl acetate
Isobutyl acetate
sec-Butyl acetate
Isopentyl acetate
Hexyl acetate
Methyl formate
Propyl formate
Ethyl propanoate
Propyl propanoate
Isobutyl propanoate
Propyl butanoate
Butyl butanoate
Ethyl 2-methylpropanoate
Isobutyl 2-methylpropanoate
Methyl 2,2-dimethylpropanoate
Ethyl 3-methylbutanoate
Methyl benzoate
Nitromethane
Propan-2-ol
Butan-1-ol
2-Butanol
2-Methylpropan-1-ol
3-Methyl-1-butanol

tert-Butanol
Pentan-1-ol
Hexan-3-ol
4-Methyl-2-pentanol
Heptane-2-ol
Heptan-4-ol
Octan-1-ol
Dodecan-1-ol
Cyclopentanol
Cyclohexanol
Propan-1,3-diol
Butan-1,4-diol
2-Methoxyethanol
2-Ethoxyethanol
2-Butoxyethanol
o-Xylene
m-Xylene
p-Xylene
Propylbenzene
1,2,3-Trimethylbenzene
1,3,5-Trimethylbenzene
Pentylbenzene
Fluorobenzene
Chlorobenzene
1,3,5-Trichlorobenzene
1,2,3,4-Tetrachlorobenzene
Pentachlorobenzene
Phenylmethylether
2-Ethylaniline
4-Ethylaniline
2,4-Dimethylaniline
2,5-Dimethylaniline
2,6-Dimethylaniline
N,N-Diethylaniline
2-Nitrotoluene
3-Nitrotoluene
2-Methylphenol
4-Methylphenol
4-tert-Butylphenol
3-Chlorophenol
3-Cyanophenol
3-Nitrophenol
1-Methylnaphthalene
2-Methylnaphthalene
Propanal
Heptanal
Octanal
Isobutyl aldehyde
3-Hydroxybenzaldehyde

2-Pentanol
3-Pentanol
Hexan-1-ol
2-Methyl-2-butanol
Heptan-1-ol
Cycloheptanol
Ethan-1,2-diol
Glycerol
2-Propoxyethanol
Benzene
Toluene
Ethylbenzene
Isopropylbenzene
1,2,4-Trimethylbenzene
4-Isopropyltoluene
Butylbenzene
Hexylbenzene
1,4-Diethylbenzene
Styrene
1,2-Dichlorobenzene
1,3-Dichlorobenzene
1,4-Dichlorobenzene
1,2,3-Trichlorobenzene
2-Chlorotoluene
3-Chlorotoluene
4-Chlorotoluene
Bromobenzene
Aniline
N,N-Dimethylaniline
Nitrobenzene
Phenol
3-Methylphenol
4-Cyanophenol
2-Nitrophenol
4-Nitrophenol
Biphenyl
Naphthalene
Acenaphthene
Fluorene
Pentanal
Hexanal
Benzaldehyde
Acetonitrile
Butyronitrile
2-Cyanopropane
2,2,2-Trifluoroethanol
2,2,3,3-Tetrafluoropropan-1-ol
1,1,1,3,3,3-Hexafluoropropan-2-ol
Methylamine

Propionitrile	Ethylamine
Pentanenitrile	Butylamine
1,2-Dicyanoethane	Pentylamine
1,3-Dicyanopropane	Hexylamine
1,4-Dicyanobutane	Diethylamine
Benzonitrile	Dipropylamine
1,1,1-Trifluoropropan-2-ol	Trimethylamine
2,2,3,3,3-Pentafluoropropan-1-ol	1,2-Diaminoethane
Propylamine	Piperidine
Isopropylamine	N-Methylpiperidine
sec-Butylamine	pyridine
tert-Butylamine	4-Ethylpyridine
Dimethylamine	2,3-Dimethylpyridine
Dibutylamine	2,6-Dimethylpyridine
Triethylamine	3,4-Dimethylpyridine
1,3-Diaminopropane	3,5-Dimethylpyridine
1,4-Diaminobutane	3-Chloropyridine
1,5-Diaminopentane	Quinoline
2-Methylpyridine	Methanethiol
3-Methylpyridine	Dimethylsulfide
4-Methylpyridine	Acetic acid
3-Ethylpyridine	Propanoic acid
2,4-Dimethylpyridine	Butanoic acid
2,5-Dimethylpyridine	Helium
2-Chloropyridine	Neon
Ethanethiol	Argon
1-Propanethiol	Krypton
1-Butanethiol	Xenon
Diethylsulfide	Radon
Dipropyl sulfide	Hydrogen
Thiophene	Nitric Oxide
2-Methoxyphenol	Carbon Dioxide
Oxygen	Benzyl alcohol
Nitrogen	2-Chlorobiphenyl
Nitrous Oxide	2,4'-Dichlorobiphenyl
Carbon Monoxide	2,5-Dichlorobiphenyl
2,3-Dichlorobiphenyl	1,2-Dimethoxyethane
2,4-Dichlorobiphenyl	Morpholine
Isophorone	Propanamide
N-Methylmorpholine	Dimethyl sulfoxide
N,N-Dimethylformamide	cis 1,2-Cyclohexanediol

Training → $\Delta_{\text{Solv}}H_W^\circ$ (kJ/mole) = - 13.572(0.635) + 9.211(1.174)**E** + 1.748(1.003)**S** - 31.460(1.561)**A** - 41.665(1.103)**B** - 6.008(0.280)**L**

(with N = 184, SD = 3.58, $R^2 = 0.967$, $R^2_{\text{adj}} = 0.966$, F = 1029.4)

Test → SD = 3.83, AAE = 3.19, AE = -0.1574

Table S5. Second Training and Test Set Analyses for Water Data Set

Training Set 2	Test Set 2
Chlorine gas	Hydrogen sulfide
Chlorine dioxide	Hydrogen selenide
2-Methylpropane	Sulphur hexafluoride
Pentane	Ammonia
2,2-Dimethylpropane	Methane
Hexane	Ethane
3-Methylpentane	Propane
2,2,4-Trimethylpentane	Butane
Cyclopropane	2-Methylpentane
Cyclohexane	2,3-Dimethylbutane
Cyclooctane	Heptane
Propene	Octane
1-Hexene	2,3,4-Trimethylpentane
2-Methylpropene	Cyclopentane
Cyclohexene	cis-1,2-Dimethylcyclohexane
Propyne	trans-1,2-Dimethylcyclohexane
Fluoromethane	Ethylcyclohexane
1,1-Difluoroethane	Ethene
1,1,1,2-Tetrafluoroethane	1-Butene
Chloromethane	1-Octene
Dichloromethane	2-Methyl-2-butene
1,1-Dichloroethane	1,3-Butadiene
1,1,2-Trichloroethane	Cyclooctene
1,1,2,2-Tetrachloroethane	1-Butyne
1-Chloropropane	Difluoromethane
1,2-Dichloropropane	Tetrafluoromethane
1,3-Dichloropropane	Trifluoromethane
1-Chlorobutane	Pentafluoroethane
1-Chloropentane	1,1,1,2,3,3,3-Heptafluoropropane
Hexafluoropropene	Trichloromethane
1,1-Dichloroethylene	Tetrachloromethane
cis-1,2-Dichloroethylene	Chloroethane
Trichloroethylene	1,2-Dichloroethane
Dibromomethane	1,1,1-Trichloroethane
Bromoethane	1,1,1,2-Tetrachloroethane
2-Methyl-2-bromopropane	2-Chlorobutane
Iodomethane	1-Chlorohexane
Iodoethane	Tetrafluoroethene
1-Iodopropane	trans-1,2-Dichloroethylene
2-Iodopropane	Bromomethane
Fluorochloromethane	Tribromomethane
Bromodichloromethane	Diiodomethane
Chlorodibromomethane	Difluorochloromethane
Dimethyl ether	Fluorotrichloromethane
Diethyl ether	Difluorodichloromethane

Di-isopropyl ether
Methyl propyl ether
Ethyl butyl ether
Methyl tert-butyl ether
Ethyl tert-butyl ether
Methyl tert-pentyl ether
Tetrahydrofuran
1,2-Diethoxyethane
1-methoxy-2-propoxyethane
2,5,8,11,14-pentaoxopentadecane
12-Crown-4
Methoxyflurane
Pentan-2-one
Pentan-3-one
Hexan-2-one
4-Methylpentan-2-one
Methyl isopropyl ketone
3,3-Dimethyl-2-butanone
Diisopropyl ketone
Heptan-2-one
Heptan-4-one
Nonan-2-one
Nonan-5-one
Propiophenone
Methyl acetate
Ethyl acetate
Propyl acetate
Butyl acetate
Isobutyl acetate
sec-Butyl acetate
tert-Butyl acetate
Pentyl acetate
Hexyl acetate
Propyl formate
Isopropyl formate
Isobutyl formate
Methyl propanoate
Butyl propanoate
Ethyl butanoate
Isobutyl 2-methylpropanoate
Methyl 2,2-dimethylpropanoate
Ethyl hexanoate
Methyl benzoate
Nitroethane
1-Nitropropane
Methanol
Propan-1-ol
Propan-2-ol
Butan-1-ol

1,1,2-Trichlorotrifluoroethane
1,2-Dichlorotetrafluoroethane
Di-n-propyl ether
Dibutyl ether
2,5-Dimethyltetrahydrofuran
2-Methyltetrahydrofuran
Tetrahydropyran
1,4-Dioxane
1,2-Dimethoxyethane
1-methoxy-2-ethoxyethane
1,2-dipropoxyethane
3,6,9-trioxoundecane
2,5,8,11-tetraoxododecane
15-Crown-5
18-Crown-6
Isoflurane
Propanone
Butanone
Hexan-3-one
Octan-2-one
Cyclopentanone
Cyclohexanone
Acetophenone
Isopropyl acetate
Isopentyl acetate
Methyl formate
Ethyl formate
Pentyl formate
3-Methylbutyl formate
Ethyl propanoate
Propyl propanoate
Isobutyl propanoate
Methyl butanoate
Propyl butanoate
Butyl butanoate
Methyl 2-methylpropanoate
Ethyl 2-methylpropanoate
Methyl pentanoate
Ethyl pentanoate
Ethyl 2,2-dimethylpropanoate
Ethyl 3-methylbutanoate
Ethyl 2-methylbutanoate
Methyl hexanoate
Nitromethane
2-Nitropropane
Ethanol
tert-Butanol
Pentan-1-ol
3-Pentanol

2-Butanol
2-Methylpropan-1-ol
3-Methyl-1-butanol
2-Pentanol
4-Methyl-2-pentanol
Heptan-1-ol
Heptane-2-ol
Heptan-4-ol
Butan-1,4-diol
2-Methoxyethanol
2-Butoxyethanol
Benzene
p-Xylene
Isopropylbenzene
1,2,4-Trimethylbenzene
1,3,5-Trimethylbenzene
Pentylbenzene
1,4-Diethylbenzene
Styrene
Fluorobenzene
1,2-Dichlorobenzene
1,4-Dichlorobenzene
1,3,5-Trichlorobenzene
1,2,3,4-Tetrachlorobenzene
2-Chlorotoluene
3-Chlorotoluene
Phenylmethylether
Aniline
2,4-Dimethylaniline
2,6-Dimethylaniline
N,N-Dimethylaniline
Nitrobenzene
3-Nitrotoluene
Phenol
3-Methylphenol
4-tert-Butylphenol
2-Nitrophenol
3-Nitrophenol
Biphenyl
Naphthalene
1-Methylnaphthalene
Acenaphthene
Fluorene
Heptanal
Benzaldehyde
Acetonitrile
Propionitrile
Pentanenitrile
2-Cyanopropane

Hexan-1-ol
Hexan-3-ol
2-Methyl-2-butanol
Octan-1-ol
Dodecan-1-ol
Cyclopentanol
Cyclohexanol
Cycloheptanol
Ethan-1,2-diol
Propan-1,3-diol
Glycerol
2-Ethoxyethanol
2-Propoxyethanol
Toluene
Ethylbenzene
o-Xylene
m-Xylene
Propylbenzene
1,2,3-Trimethylbenzene
4-Isopropyltoluene
Butylbenzene
Hexylbenzene
Chlorobenzene
1,3-Dichlorobenzene
1,2,3-Trichlorobenzene
Pentachlorobenzene
4-Chlorotoluene
Bromobenzene
2-Ethylaniline
4-Ethylaniline
2,5-Dimethylaniline
N,N-Diethylaniline
2-Nitrotoluene
2-Methylphenol
4-Methylphenol
3-Chlorophenol
3-Cyanophenol
4-Cyanophenol
4-Nitrophenol
2-Methylnaphthalene
Propanal
Pentanal
Hexanal
Octanal
Isobutyl aldehyde
3-Hydroxybenzaldehyde
Butyronitrile
Benzonitrile
2,2,2-Trifluoroethanol

1,2-Dicyanoethane	1,1,1-Trifluoropropan-2-ol
1,3-Dicyanopropane	2,2,3,3-Tetrafluoropropan-1-ol
1,4-Dicyanobutane	2,2,3,3,3-Pentafluoropropan-1-ol
1,1,1,3,3,3-Hexafluoropropan-2-ol	Ethylamine
Methylamine	Butylamine
Propylamine	sec-Butylamine
Isopropylamine	tert-Butylamine
Pentylamine	Diethylamine
Hexylamine	Dipropylamine
Dimethylamine	Dibutylamine
1,2-Diaminoethane	Trimethylamine
1,3-Diaminopropane	Triethylamine
1,4-Diaminobutane	N-Methylpiperidine
1,5-Diaminopentane	2-Methylpyridine
Piperidine	3-Methylpyridine
Pyridine	3,5-Dimethylpyridine
4-Methylpyridine	3-Chloropyridine
3-Ethylpyridine	Quinoline
4-Ethylpyridine	Ethanethiol
2,3-Dimethylpyridine	1-Butanethiol
2,4-Dimethylpyridine	Dimethylsulfide
2,5-Dimethylpyridine	Diethylsulfide
2,6-Dimethylpyridine	Dipropyl sulfide
3,4-Dimethylpyridine	Acetic acid
2-Chloropyridine	Propanoic acid
Methanethiol	2-Methoxyphenol
1-Propanethiol	Neon
Thiophene	Xenon
Butanoic acid	Oxygen
Helium	Nitrogen
Argon	Carbon Monoxide
Krypton	Carbon Dioxide
Radon	2,4-Dichlorobiphenyl
Hydrogen	2,4'-Dichlorobiphenyl
Nitrous Oxide	2,5-Dichlorobiphenyl
Nitric Oxide	1,2-Dimethoxyethane
Benzyl alcohol	Isophorone
2-Chlorobiphenyl	Morpholine
2,3-Dichlorobiphenyl	N-Methylmorpholine
Propanamide	Dimethyl sulfoxide
N,N-Dimethylformamide	cis 1,2-Cyclohexanediol

Training $\rightarrow \Delta_{\text{Solv}}H_{\text{W}}$ (kJ/mole) = - 13.056(0.688) + 10.459(1.140)**E** + 1.876(1.044)**S** - 33.656(1.750)**A** - 40.997(1.170)**B** - 6.340(0.307)**L**

(with N = 184, SD = 3.69, $R^2 = 0.959$, $R^2_{\text{adj}} = 0.958$, F = 832.6)

Test \rightarrow SD = 3.71, AAE = 2.93, AE = -0.1830

Table S6. Second Training and Test Set Analyses for Water Data Set

Training Set 3	Test Set 3
Hydrogen sulfide	Chlorine gas
Hydrogen selenide	Sulphur hexafluoride
Chlorine dioxide	Methane
Ammonia	Propane
Ethane	Butane
2-Methylpropane	Pentane
2-Methylpentane	2,2-Dimethylpropane
3-Methylpentane	Hexane
2,3-Dimethylbutane	Octane
Heptane	Cyclopropane
2,2,4-Trimethylpentane	Cyclohexane
2,3,4-Trimethylpentane	Cyclooctane
Cyclopentane	Ethene
cis-1,2-Dimethylcyclohexane	1-Butene
trans-1,2-Dimethylcyclohexane	1-Hexene
Ethylcyclohexane	1,3-Butadiene
Propene	Cyclohexene
1-Octene	Fluoromethane
2-Methylpropene	1,1-Difluoroethane
2-Methyl-2-butene	Trifluoromethane
Cyclooctene	1,1,1,2,3,3,3-Heptafluoropropane
Propyne	Dichloromethane
1-Butyne	Trichloromethane
Difluoromethane	Tetrachloromethane
Tetrafluoromethane	Chloroethane
1,1,1,2-Tetrafluoroethane	1,1-Dichloroethane
Pentafluoroethane	1,2-Dichloroethane
Chloromethane	1,1,1-Trichloroethane
1,1,2,2-Tetrachloroethane	1,1,2-Trichloroethane
2-Chlorobutane	1,1,1,2-Tetrachloroethane
1-Chloropentane	1-Chloropropane
cis-1,2-Dichloroethylene	1,2-Dichloropropane
trans-1,2-Dichloroethylene	1,3-Dichloropropane
Trichloroethylene	1-Chlorobutane
2-Methyl-2-bromopropane	1-Chlorohexane
Iodomethane	Tetrafluoroethene
1-Iodopropane	Hexafluoropropene
2-Iodopropane	1,1-Dichloroethylene
Fluorochloromethane	Bromomethane
Bromodichloromethane	Dibromomethane
Difluorodichloromethane	Tribromomethane
1,2-Dichlorotetrafluoroethane	Bromoethane
Dimethyl ether	Diiodomethane
Tetrahydropyran	Iodoethane
1,4-Dioxane	Difluorochloromethane
1-methoxy-2-ethoxyethane	Chlorodibromomethane

1-methoxy-2-propoxyethane
2,5,8,11-tetraoxododecane
2,5,8,11,14-pentaoxopentadecane
15-Crown-5
Methoxyflurane
Butanone
Pentan-3-one
Hexan-2-one
4-Methylpentan-2-one
Methyl isopropyl ketone
Diisopropyl ketone
Heptan-4-one
Nonan-2-one
Cyclohexanone
Acetophenone
Propiophenone
Methyl acetate
Ethyl acetate
tert-Butyl acetate
Ethyl formate
Propyl formate
Isobutyl formate
Ethyl propanoate
Butyl propanoate
Isobutyl propanoate
Methyl butanoate
Ethyl butanoate
Propyl butanoate
Methyl 2-methylpropanoate
Isobutyl 2-methylpropanoate
Methyl pentanoate
Ethyl 2-methylbutanoate
Methyl hexanoate
Ethyl hexanoate
Methyl benzoate
Nitromethane
Nitroethane
Ethanol
Propan-2-ol
Butan-1-ol
2-Butanol
2-Methylpropan-1-ol
tert-Butanol
3-Methyl-1-butanol
3-Pentanol
Hexan-3-ol
2-Methyl-2-butanol
4-Methyl-2-pentanol
Heptan-1-ol

Fluorotrichloromethane
1,1,2-Trichlorotrifluoroethane
Diethyl ether
Di-n-propyl ether
Di-isopropyl ether
Dibutyl ether
Methyl propyl ether
Ethyl butyl ether
Methyl tert-butyl ether
Ethyl tert-butyl ether
Methyl tert-pentyl ether
Tetrahydrofuran
2,5-Dimethyltetrahydrofuran
2-Methyltetrahydrofuran
1,2-Dimethoxyethane
1,2-Diethoxyethane
1,2-dipropoxyethane
3,6,9-trioxoundecane
12-Crown-4
18-Crown-6
Isoflurane
Propanone
Pentan-2-one
Hexan-3-one
3,3-Dimethyl-2-butanone
Heptan-2-one
Octan-2-one
Nonan-5-one
Cyclopentanone
Propyl acetate
Isopropyl acetate
Butyl acetate
Isobutyl acetate
sec-Butyl acetate
Pentyl acetate
Isopentyl acetate
Hexyl acetate
Methyl formate
Isopropyl formate
Pentyl formate
3-Methylbutyl formate
Methyl propanoate
Propyl propanoate
Butyl butanoate
Ethyl 2-methylpropanoate
Ethyl pentanoate
Methyl 2,2-dimethylpropanoate
Ethyl 2,2-dimethylpropanoate
Ethyl 3-methylbutanoate

Heptan-4-ol
Cyclohexanol
2-Ethoxyethanol
Benzene
Toluene
Ethylbenzene
m-Xylene
p-Xylene
Propylbenzene
1,2,3-Trimethylbenzene
1,3,5-Trimethylbenzene
4-Isopropyltoluene
Pentylbenzene
1,4-Diethylbenzene
Styrene
Chlorobenzene
1,2-Dichlorobenzene
1,3-Dichlorobenzene
1,2,3-Trichlorobenzene
1,3,5-Trichlorobenzene
1,2,3,4-Tetrachlorobenzene
Pentachlorobenzene
Bromobenzene
Aniline
2-Ethylaniline
2,6-Dimethylaniline
N,N-Dimethylaniline
N,N-Diethylaniline
2-Nitrotoluene
3-Methylphenol
4-Methylphenol
4-tert-Butylphenol
3-Cyanophenol
4-Nitrophenol
2-Methylnaphthalene
Fluorene
Propanal
Hexanal
Octanal
Isobutyl aldehyde
Butyronitrile
Pentanenitrile
2-Cyanopropane
1,2-Dicyanoethane
1,4-Dicyanobutane
Benzonitrile
2,2,2-Trifluoroethanol
1,1,1,3,3,3-Hexafluoropropan-2-ol
Methylamine

1-Nitropropane
2-Nitropropane
Methanol
Propan-1-ol
Pentan-1-ol
2-Pentanol
Hexan-1-ol
Heptane-2-ol
Octan-1-ol
Dodecan-1-ol
Cyclopentanol
Cycloheptanol
Ethan-1,2-diol
Propan-1,3-diol
Butan-1,4-diol
Glycerol
2-Methoxyethanol
2-Propoxyethanol
2-Butoxyethanol
o-Xylene
Isopropylbenzene
1,2,4-Trimethylbenzene
Butylbenzene
Hexylbenzene
Fluorobenzene
1,4-Dichlorobenzene
2-Chlorotoluene
3-Chlorotoluene
4-Chlorotoluene
Phenylmethylether
4-Ethylaniline
2,4-Dimethylaniline
2,5-Dimethylaniline
Nitrobenzene
3-Nitrotoluene
Phenol
2-Methylphenol
3-Chlorophenol
4-Cyanophenol
2-Nitrophenol
3-Nitrophenol
Biphenyl
Naphthalene
1-Methylnaphthalene
Acenaphthene
Pentanal
Heptanal
Benzaldehyde
3-Hydroxybenzaldehyde

Ethylamine	Acetonitrile
Isopropylamine	Propionitrile
tert-Butylamine	1,3-Dicyanopropane
Dipropylamine	1,1,1-Trifluoropropan-2-ol
Triethylamine	2,2,3,3-Tetrafluoropropan-1-ol
1,4-Diaminobutane	2,2,3,3,3-Pentafluoropropan-1-ol
Piperidine	Propylamine
N-Methylpiperidine	Butylamine
pyridine	sec-Butylamine
3-Ethylpyridine	Pentylamine
2,6-Dimethylpyridine	Hexylamine
3,5-Dimethylpyridine	Dimethylamine
2-Chloropyridine	Diethylamine
Ethanethiol	Dibutylamine
1-Propanethiol	Trimethylamine
1-Butanethiol	1,2-Diaminoethane
Dimethylsulfide	1,3-Diaminopropane
Diethylsulfide	1,5-Diaminopentane
Dipropyl sulfide	2-Methylpyridine
Acetic acid	3-Methylpyridine
Butanoic acid	4-Methylpyridine
2-Methoxyphenol	4-Ethylpyridine
Helium	2,3-Dimethylpyridine
Neon	2,4-Dimethylpyridine
Xenon	2,5-Dimethylpyridine
Radon	3,4-Dimethylpyridine
Oxygen	3-Chloropyridine
Nitrogen	Quinoline
Nitrous Oxide	Methanethiol
Nitric Oxide	Thiophene
Carbon Monoxide	Propanoic acid
Carbon Dioxide	Argon
2-Chlorobiphenyl	Krypton
2,4'-Dichlorobiphenyl	Hydrogen
2,5-Dichlorobiphenyl	Benzyl alcohol
1,2-Dimethoxyethane	2,3-Dichlorobiphenyl
Isophorone	2,4-Dichlorobiphenyl
Morpholine	N-Methylmorpholine
Propanamide	N,N-Dimethylformamide
cis 1,2-Cyclohexanediol	Dimethyl sulfoxide

Training → $\Delta_{\text{Solv}}H_{\text{W}}$ (kJ/mole) = - 13.311(0.612) + 11.645(1.185)**E** + 3.335(1.130)**S** - 33.355(1.632)**A** - 41.349(1.182)**B** - 6.665(0.277)**L**

(with N = 184, SD = 3.63, $R^2 = 0.964$, $R^2_{\text{adj}} = 0.963$, F = 940.9)

Test → SD = 3.81, AAE = 3.00, AE = 0.0737