Fast and accurate calculation of hydration energies of molecules and ions

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Supplementary Materials

GEPOL93[1] default parameters used in our calculations:

Division level for the triangles on the surface, NDIV=3
Overlapping factor, OFAC=0.8
Radius of the smallest sphere, R_{min}=0.5 Å
Solvent radius, R_{solv} =1.4 Å

Table S1. Cations: 60-set from Ref. 31

			ΔG°_{solv}, kcal/mol						
			expe-	B3LYP/Def2TZVP			B3LYP/6-31G*		
Code			rimen-tal	SMD	PCM	xESE	SMD	PCM	xESE
c047	H_6NO^+	ammonia	-74.6	-71.7	-62.4	-78.770	-70.950	-62.074	-78.971
c050	$H_7CO_2^+$	methanol	-76.6	-69.3	-58.2	-74.198	-68.736	-58.183	-74.359
c051	$H_9C_2O_2^+$	ethanol	-73.6	-66.6	-55.6	-69.058	-66.119	-55.537	-69.306
c052	$H_9C_2O_2^+$	dimethylether	-66.3	-61.1	-53.1	-63.380	-60.485	-52.929	-63.414
c053	$H_{13}C_4O_2^+$	diethylether	-62.2	-57.2	-49.5	-56.985	-56.618	-49.385	-57.099
c054	$H_9C_3O_2^+$	acetone	-66.3	-60.5	-52.0	-61.694	-60.100	-51.938	-61.913
c056	$H_{11}C_8O_2^+$	acetophenone	-55.7	-52.7	-45.2	-52.497	-52.190	-45.055	-52.930
c088	$H_5O_2^+$	water Zundel ion	-87.8	-78.7	-64.1	-83.697	-78.025	-64.084	-83.823
i003	H_6CN^+	methylamine	-76.4	-74.4	-65.7	-83.922	-74.086	-65.715	-84.015
i004	$H_{10}C_3N^+$	n-propylamine	-71.5	-70.0	-61.2	-74.262	-69.645	-61.221	-74.552
i005	$H_{10}C_3N^+$	isopropylamine	-69.6	-68.7	-59.9	-72.028	-68.265	-59.849	-72.262
i006	$H_{12}C_4N^+$	tert-butylamine	-67.3	-66.3	-57.4	-68.051	-65.813	-57.389	-68.324
i007	$H_{14}C_6N^+$	cyclohexanamine	-68.7	-66.2	-56.9	-66.906	-65.801	-56.931	-67.280
i008	$H_8C_3N^+$	allylamine	-72.0	-69.8	-61.2	-74.457	-69.164	-61.041	-74.696
i009	$H_8C_2N^+$	dimethylamine	-68.6	-67.7	-60.1	-73.398	-67.442	-60.117	-73.500
i010	$H_{12}C_4N^+$	diethylamine	-63.4	-62.8	-54.9	-63.399	-62.389	-54.901	-63.582
i011	$H_{16}C_6N^+$	di-n-propylamine	-60.5	-60.5	-52.8	-58.968	-59.965	-52.744	-59.263
i012	$H_{12}C_6N^+$	diallylamine	-61.6	-60.3	-52.9	-60.821	-59.378	-52.647	-61.142
i013	$H_{10}C_3N^+$	trimethylamine	-61.1	-62.0	-55.4	-61.480	-61.716	-55.423	-61.480
i014	$H_{16}C_6N^+$	triethylamine	-54.6	-55.8	-49.0	-50.296	-55.161	-48.811	-50.340
i015	$H_{22}C_9N^+$	tri-n-propylamine	-50.9	-52.9	-46.3	-45.201	-52.190	-46.167	-45.299
i018	$H_8C_6N^+$	aniline	-72.4	-68.1	-58.8	-72.688	-67.439	-58.575	-73.353
i019	$H_{10}C_7N^+$	2-methylaniline	-70.3	-66.6	-57.0	-68.480	-65.954	-56.758	-68.946
i020	$H_{10}C_7N^+$	3-methylaniline	-69.6	-65.9	-57.2	-69.145	-65.311	-57.063	-69.681
i021	$H_{10}C_7N^+$	4-methylaniline	-69.8	-65.9	-57.1	-69.169	-65.344	-57.043	-69.746
i023	$H_9C_6N_2^+$	3-aminoaniline	-65.8	-67.3	-57.2	-70.619	-66.665	-56.983	-71.261
i024	$H_{10}C_7N^+$	N-methylaniline	-62.6	-62.2	-53.8	-63.513	-61.507	-53.570	-63.850
i025	$H_{12}C_8N^+$	N-ethylaniline	-62.2	-60.1	-51.6	-59.520	-59.393	-51.340	-59.849
i026	$H_{12}C_8N^+$	N,N-dimethylaniline	-57.2	-56.9	-49.7	-57.598	-56.162	-49.374	-57.768
i027	$H_{14}C_9N^+$	4-methyl-N,N-dimethylaniline	-55.9	-54.9	-48.4	-55.340	-54.325	-48.163	-55.620
i028	$H_{16}C_{10}N^+$	N,N-diethylaniline	-54.0	-53.5	-46.3	-51.861	-52.653	-45.974	-52.012
i029	$H_{10}C_{10}N^+$	1-aminonaphthalene	-67.4	-65.5	-55.6	-66.625	-64.836	-55.287	-67.286
i030	$H_6C_2N^+$	aziridine	-70.9	-70.5	-61.2	-76.891	-70.329	-61.228	-76.947
i031	$H_8C_3N^+$	azetidine	-67.7	-66.5	-58.4	-70.593	-66.150	-58.397	-70.711
i032	$H_{10}C_4N^+$	pyrrolidine	-66.0	-64.5	-56.4	-66.927	-64.183	-56.427	-67.097
i033	$H_{12}C_5N^+$	piperidine	-64.2	-63.1	-54.7	-64.086	-62.800	-54.747	-64.318
i034	$H_{14}C_6N^+$	azacycloheptane	-63.3	-61.9	-53.2	-60.990	-61.423	-53.146	-61.236
i035	$H_6C_4N^+$	pyrrole	-61.4	-62.7	-54.9	-67.284	-62.195	-54.723	-67.386
i036	$H_6C_5N^+$	pyridine	-61.1	-59.6	-53.2	-65.799	-59.142	-53.013	-65.894
i037	$H_8C_9N^+$	quinoline	-56.0	-54.2	-47.9	-56.782	-53.522	-47.499	-56.974
i039	$H_{11}C_4N_2^+$	piperazine	-66.0	-67.0	-55.7	-67.372	-66.509	-55.611	-67.720
i040	$H_4C_2N^+$	acetonitrile	-75.3	-65.9	-60.0	-80.086	-65.611	-59.986	-80.300

i047	H_4N^+	ammonia	-85.2	-82.3	-72.7	-100.248	-82.006	-72.670	-100.225
i048	$H_5N_2^+$	hydrazine	-84.6	-80.1	-69.9	-90.936	-80.035	-70.109	-91.083
i050	H_5CO^+	methanol	-93.0	-80.5	-67.3	-91.315	-80.320	-67.432	-91.403
i051	$H_7C_2O^+$	ethanol	-88.4	-75.9	-63.1	-82.475	-75.751	-63.233	-82.695
i052	$H_7C_2O^+$	dimethylether	-79.7	-69.3	-60.0	-77.523	-69.109	-60.022	-77.630
i053	$H_{11}C_4O^+$	diethylether	-71.5	-62.7	-53.7	-65.698	-62.359	-53.743	-65.866
i054	$H_7C_3O^+$	acetone	-77.1	-67.5	-57.9	-74.110	-67.516	-58.009	-74.398
i056	$H_9C_8O^+$	acetophenone	-64.5	-56.9	-48.5	-60.103	-56.468	-48.340	-60.537
i088	H_3O^+	oxonium	-110.3	-96.2	-77.6	-110.293	-95.952	-77.650	-110.302
i093	$H_{10}C_7NO^+$	4-methoxyaniline	-71.2	-65.6	-56.9	-68.886	-65.118	-56.769	-69.552
i094	$H_7C_6N_2O_2^+$	4-nitroaniline	-75.9	-77.5	-68.5	-80.113	-76.355	-67.669	-80.663
i095	$H_{10}C_4NO^+$	morpholine	-69.6	-69.3	-58.8	-70.526	-68.929	-58.761	-70.889
i098	$H_6C_2NO^+$	acetamide	-73.9	-70.3	-60.2	-76.849	-70.134	-60.207	-77.237
i099	$H_8C_7NO^+$	benzamide	-67.2	-62.3	-52.7	-65.071	-61.932	-52.591	-65.664
i106	$H_7C_2S^+$	dimethylsulfide	-64.5	-59.2	-57.3	-67.177	-59.263	-57.733	-67.423
i112	$H_7C_2OS^+$	dimethylsulfoxide	-67.7	-60.8	-55.9	-68.415	-60.681	-56.087	-68.715
i125	$H_7C_6NCl^+$	3-chloroaniline	-74.7	-70.2	-60.6	-72.734	-70.055	-60.746	-73.591
i126	$H_7C_6NCl^+$	4-chloroaniline	-74.1	-70.4	-60.8	-73.912	-70.306	-61.018	-74.828

Subsets of cations:

Small cations:
c047, c088, i003, i040, i047, i048, i050, i088

Oxygen-containing cations:
c047, c050, c051, c052, c053, c054, c056, c088, i050, i051, i052, i053, i054, i056, i088, i093, i094, i095, i098, i099, i112

Halogen-containing cations:
i125, i126

Table S2. Anions: 83-set from Ref. 31

				ΔG°_{solv}, kcal/mol					
			expe-	B3LYP/Def2TZVP			B3LYP/6-31G*		
Code			rime-ntal	SMD	PCM	xESE	SMD	PCM	xESE
c001	$H_3C_2O^-$	acetylene·H_2O	-67.9	-65.9	-63.5	-77.014	-68.750	-64.082	-77.503
c046b	H_2CNO^-	hydrogencyanide	-64.0	-60.9	-61.6	-79.366	-63.901	-62.726	-79.557
c065	$H_5CO_2^-$	methanolate	-80.0	-72.3	-64.7	-83.230	-74.417	-64.716	-83.716
c066	$H_7C_2O_2^-$	ethanolate	-78.5	-69.8	-62.3	-78.451	-71.914	-62.299	-79.434
c067	$H_9C_3O_2^-$	1-propanolate	-75.8	-69.2	-61.7	-76.088	-71.066	-61.641	-77.037
c068	$H_9C_3O_2^-$	isopropanolate	-76.0	-67.8	-60.2	-75.529	-69.724	-60.059	-76.519
c069	$H_{11}C_4O_2^-$	2-butanolate	-76.3	-66.0	-58.6	-73.274	-68.183	-58.636	-74.331
c070	$H_{11}C_4O_2^-$	t-butanolate	-72.1	-65.9	-58.5	-72.462	-67.754	-58.275	-73.646
c071	$H_7C_3O_2^-$	allyl alcoholate	-75.1	-67.8	-60.9	-74.948	-69.633	-60.805	-75.728
c072	$H_9C_7O_2^-$	benzyl alcoholate	-75.4	-64.0	-57.4	-69.671	-65.946	-57.393	-70.736
c073	$H_9C_3O_3^-$	2-methoxyethanolate	-77.9	-69.8	-62.1	-76.180	-71.625	-61.973	-77.106
c078	$H_7C_2O_3^-$	1,2-ethanediolate	-73.3	-74.0	-63.8	-80.049	-76.266	-63.798	-81.038
c082	$H_5CO_3^-$	methylhydroperoxide	-80.6	-73.5	-64.4	-79.401	-76.111	-64.446	-80.191
c083	$H_7C_2O_3^-$	ethylhydroperoxide	-77.1	-73.1	-63.8	-77.116	-75.682	-63.750	-78.087
c089	$H_3O_2^-$	$OH^-(H_2O)$	-86.9	-83.5	-71.9	-91.677	-86.781	-71.947	-92.132
c090	$H_3O_3^-$	hydrogenperoxide	-82.3	-75.1	-65.3	-84.572	-78.565	-65.896	-85.236
c091	$H_2O_3^-$	hydroperoxylradical	-73.2	-72.0	-63.5	-78.495	-75.301	-64.172	-78.869
c111	H_3OS^-	hydrogensulfide	-65.5	-61.7	-63.2	-68.634	-62.882	-64.467	-69.006
c114	H_2OF^-	fluoride·H_2O	-85.5	-77.7	-72.4	-85.498	-79.537	-72.577	-85.503
c115	H_2OCl^-	chloride·H_2O	-67.5	-63.8	-65.1	-68.459	-64.737	-65.853	-68.670
c116	H_2OBr^-	bromide·H_2O	-63.2	-54.3	-61.3	-70.338	-55.063	-62.722	-70.667
c121	$H_4C_2O_2F_3^-$	2,2,2-trifluoroethanolate·H_2O	-68.0	-62.0	-57.1	-68.772	-63.860	-57.310	-69.260
c122	$H_3C_3O_2F_6^-$	1,1,1,3,3,3-hexafluoro-propan-2-olate·H_2O	-61.6	-55.2	-52.8	-59.520	-56.972	-53.159	-59.980
i001	HC_2^-	acetylene	-76.5	-71.4	-70.3	-93.557	-74.991	-71.382	-93.082
i041	$H_2C_2N^-$	acetonitrile	-66.6	-61.2	-62.3	-66.605	-63.580	-63.435	-66.793
i043	HCN_2^-	cyanamide	-72.2	-64.6	-65.4	-71.317	-66.163	-66.254	-71.681
i044	$H_6C_6N^-$	aniline	-62.9	-57.9	-56.4	-69.653	-59.040	-56.732	-70.181
i045	$H_{10}C_{12}N^-$	diphenylamine	-54.6	-48.1	-47.8	-59.301	-49.595	-48.494	-60.416
i046	CN^-	cyanide	-70.2	-65.1	-67.8	-72.841	-68.723	-69.743	-72.559
i058	HCO_2^-	formate	-76.2	-70.6	-66.0	-83.744	-72.909	-66.232	-83.624

i059	$H_3C_2O_2^-$	acetate	-77.6	-71.1	-65.2	-80.307	-73.209	-65.140	-80.589
i060	$H_5C_3O_2^-$	propanoate	-76.2	-69.4	-63.6	-76.894	-71.047	-63.213	-77.232
i061	$H_{11}C_6O_2^-$	hexanoate	-74.6	-67.9	-62.7	-73.209	-69.272	-62.141	-73.518
i062	$H_3C_3O_2^-$	acrylate	-74.0	-67.9	-63.2	-76.234	-69.705	-62.978	-76.274
i063	$H_3C_3O_3^-$	pyruvate	-68.5	-64.9	-60.7	-71.978	-66.704	-60.588	-72.199
i064	$H_5C_7O_2^-$	benzoate	-71.2	-64.5	-59.8	-69.619	-65.965	-59.385	-69.688
i065	H_3CO^-	methanolate	-95.0	-79.5	-70.7	-95.229	-80.788	-70.482	-95.127
i066	$H_5C_2O^-$	ethanolate	-90.7	-75.5	-67.0	-88.777	-76.937	-66.857	-89.291
i067	$H_7C_3O^-$	1-propanolate	-88.3	-74.6	-66.1	-85.590	-75.668	-65.665	-86.046
i068	$H_7C_3O^-$	isopropanolate	-86.3	-72.7	-64.4	-84.271	-73.898	-64.028	-85.053
i069	$H_9C_4O^-$	2-butanolate	-84.2	-69.5	-61.7	-80.621	-70.698	-61.342	-81.574
i070	$H_9C_4O^-$	t-butanolate	-82.3	-70.7	-62.4	-80.987	-71.459	-61.702	-81.814
i071	$H_5C_3O^-$	allyl alcoholate	-86.6	-73.1	-65.4	-84.692	-73.998	-64.811	-84.725
i072	$H_7C_7O^-$	benzyl alcoholate	-85.1	-67.8	-60.5	-76.964	-68.691	-60.069	-77.313
i073	$H_7C_3O_2^-$	2-methoxyethanol	-89.4	-75.4	-66.8	-86.161	-76.375	-66.212	-86.503
i074	$H_5C_6O^-$	phenolate	-71.9	-60.9	-57.1	-70.705	-62.290	-57.136	-70.871
i075	$H_7C_7O^-$	2-methylphenolate	-70.2	-59.1	-55.4	-68.853	-60.395	-55.453	-69.291
i076	$H_7C_7O^-$	3-methylphenolate	-71.1	-60.3	-56.7	-69.626	-61.488	-56.670	-69.851
i077	$H_7C_7O^-$	4-methylphenolate	-72.0	-60.3	-56.6	-69.431	-61.195	-56.362	-69.446
i078	$H_5C_2O_2^-$	1,2-ethanediolate	-85.3	-80.7	-69.5	-89.287	-82.060	-69.099	-89.596
i080	$H_5C_6O_2^-$	3-hydroxyphenolate	-73.8	-63.7	-57.9	-72.527	-65.341	-57.997	-72.978
i081	$H_5C_6O_2^-$	4-hydroxyphenolate	-77.6	-66.1	-59.3	-73.737	-67.413	-59.126	-73.959
i082	$H_3CO_2^-$	methylhydroperoxide	-93.2	-83.1	-71.9	-92.759	-85.586	-71.729	-93.260
i083	$H_5C_2O_2^-$	ethylhydroperoxide	-89.2	-82.3	-71.0	-89.661	-84.605	-70.614	-90.332
i084	$H_3C_2O^-$	acetaldehyde	-76.5	-67.1	-63.6	-83.159	-69.522	-64.136	-83.466
i085	$H_5C_3O^-$	acetone	-76.2	-66.1	-62.2	-79.643	-68.298	-62.541	-80.429
i086	$H_9C_5O^-$	3-pentanone	-73.7	-61.5	-57.3	-73.213	-63.232	-57.540	-74.291
i089	HO^-	hydroxide	-104.7	-101.8	-85.7	-104.697	-106.033	-85.508	-104.751
i090	HO_2^-	hydrogenperoxide	-97.3	-93.0	-78.4	-90.294	-96.888	-78.583	-90.623
i091	O_2^-	hydroperoxyl radical	-83.3	-83.2	-73.3	-86.578	-87.636	-74.385	-86.578
i100	$H_4C_6NO_3^-$	2-nitrophenol	-60.1	-55.1	-53.3	-61.630	-56.411	-53.188	-61.732
i101	$H_4C_6NO_3^-$	3-nitrophenol	-61.9	-51.7	-50.7	-60.706	-52.825	-50.542	-60.620
i102	$H_4C_6NO_3^-$	4-nitrophenol	-57.8	-49.6	-48.9	-58.390	-50.743	-48.799	-58.417
i103	$H_2CNO_2^-$	nitromethane	-76.5	-65.9	-63.3	-83.976	-67.856	-63.524	-84.188
i104	$H_5C_6N_2O_2^-$	4-nitroaniline	-57.4	-50.3	-49.4	-58.999	-51.237	-49.564	-59.387
i105	$H_4C_2NO^-$	acetamide	-80.2	-68.7	-63.7	-79.002	-70.341	-63.925	-79.584
i107	H_3CS^-	methanethiol	-73.8	-61.1	-68.2	-74.280	-62.140	-69.818	-74.663
i108	$H_5C_2S^-$	ethanethiol	-71.8	-58.7	-65.5	-70.765	-59.993	-67.444	-71.680
i109	$H_7C_3S^-$	1-propanethiol	-70.5	-58.0	-65.1	-68.415	-59.197	-66.857	-69.346
i110	$H_5C_6S^-$	thiophenol	-63.4	-52.7	-57.1	-62.399	-54.069	-58.792	-63.284
i111	HS^-	hydrogensulfide	-72.1	-65.0	-71.0	-72.087	-65.545	-72.246	-71.816
i113	$H_5C_2OS^-$	dimethylsulfoxide	-67.7	-62.9	-60.9	-78.076	-64.539	-61.539	-79.178
i114	F^-	fluoride	-104.4	-91.2	-87.6	-116.076	-92.838	-88.518	-116.076
i115	Cl^-	chloride	-74.5	-67.3	-72.9	-74.481	-67.588	-73.537	-74.481
i116	Br^-	bromide	-68.3	-53.9	-67.3	-68.305	-54.097	-69.554	-68.305
i117	CCl_3^-	chloroform	-54.1	-49.1	-52.9	-61.905	-49.347	-53.203	-61.846
i118	$C_2O_2F_3^-$	trifluoroacetate	-59.3	-58.3	-57.3	-66.555	-60.920	-58.038	-66.642
i119	$H_2C_2O_2Cl^-$	chloroacetate	-69.7	-64.5	-60.4	-72.685	-65.632	-60.180	-72.587
i120	$HC_2O_2Cl_2^-$	dichloroacetate	-62.3	-60.1	-57.0	-68.741	-60.854	-56.693	-68.496
i121	$H_2C_2OF_3^-$	2,2,2-trifluoroethanolote	-77.5	-66.6	-61.5	-77.761	-67.670	-61.378	-77.728
i122	$HC_3OF_6^-$	1,1,1,3,3,3-hexafluoropropan-2-olate	-65.5	-57.4	-55.5	-65.696	-58.696	-55.623	-65.884
i123	$H_4C_6OCl^-$	2-chlorophenolate	-66.1	-56.7	-54.5	-66.699	-57.642	-54.649	-66.850
i124	$H_4C_6OCl^-$	4-chlorophenolate	-66.0	-55.9	-53.0	-65.646	-56.591	-52.771	-65.555

Subsets of anions:

Small anions:
c001, c046b, c065, c089, c090, c091, c111, c114, c115, c116, i001, i041, i043, i046, i058, i059, i062, i065, i066, i082, i084, i089, i090, i091, i103, i105, i107, i108, i111, i114, i115, i116, i117, i118, i119, i120, i121

Oxygen-containing anions:
c001, c046b, c065, c066, c067, c068, c069, c070, c071, c072, c073, c078, c082, c083, c089, c090, c091, c111, c114, c115, c116, c121, c122, i058, i059, i060, i061, i062, i063, i064, i065, i066, i067, i068, i069,

i070, i071, i072, i073, i074, i075, i076, i077, i078, i080, i081, i082, i083, i084, i085, i086, i089, i090, i091, i100, i101, i102, i103, i104, i105, i113, i118, i119, i120, i121, i122, i123, i124

Halogen-containing anions:
c114, c115, c116, c121, c122, i114, i115, i116, i117, i118, i119, i120, i121, i122, i123, i124

Training set for ions:
i006, i010, i013, i018, i020, i021, i026, i027, i033, i041, i060, i065, i082, i083, i086, i088, i089, i102, i107, i111, i112, i115, i116, i121, i122, i123, i124, i126, c066, c067, c068, c070, c071, c083, c114

Table S3. Neutral molecules: 390-set from Ref. 31

	Name		ΔG°_{solv}, kcal/mol						
			experi-	B3LYP/Def2TZVP			B3LYP/6-31G*		
Code			mental	SMD	PCM	xESE	SMD	PCM	xESE
0001met	H_4C	methane	2.00	2.20	-0.12	0.674	2.288	-0.108	0.670
0002eth	H_6C_2	ethane	1.83	1.79	-0.11	0.873	1.925	-0.091	0.862
0003pro	H_8C_3	n-propane	1.96	1.83	-0.15	1.097	2.007	-0.113	1.083
0004nbu	$H_{10}C_4$	n-butane	2.08	2.01	-0.18	1.262	2.218	-0.131	1.242
0005npe	$H_{12}C_5$	n-pentane	2.33	2.18	-0.21	1.477	2.422	-0.148	1.454
0006nhe	$H_{14}C_6$	n-hexane	2.49	2.36	-0.23	1.647	2.635	-0.166	1.622
0007nhe	$H_{16}C_7$	n-heptane	2.62	2.54	-0.26	1.850	2.844	-0.182	1.820
0008noc	$H_{18}C_8$	n-octane	2.89	2.71	-0.29	0.139	3.056	-0.202	0.072
0010met	$H_{10}C_4$	2-methylpropane	2.32	2.05	-0.20	1.263	2.291	-0.153	1.245
0011dim	$H_{12}C_5$	2,2-dimethylpropane	2.50	2.25	-0.30	1.468	2.557	-0.219	1.453
0012met	$H_{14}C_6$	2-methylpentane	2.52	2.38	-0.25	1.724	2.688	-0.178	1.702
0013dim	$H_{16}C_7$	2,4-dimethylpentane	2.88	2.65	-0.31	1.930	3.010	-0.224	1.905
0014tri	$H_{18}C_8$	2,2,4-trimethylpentane	2.85	2.73	-0.38	2.109	3.174	-0.275	2.087
0016cyc	H_6C_3	cyclopropane	0.75	0.07	-0.62	0.516	0.137	-0.619	0.468
0017cyc	$H_{10}C_5$	cyclopentane	1.20	1.26	-0.18	1.196	1.452	-0.134	1.161
0018cyc	$H_{12}C_6$	cyclohexane	1.23	1.35	-0.15	1.583	1.569	-0.105	1.558
0019met	$H_{14}C_7$	methylcyclohexane	1.71	1.75	-0.20	1.711	2.012	-0.145	1.686
0020cis	$H_{16}C_8$	cis-1,2-dimethylcyclohexane	1.58	1.97	-0.25	1.998	2.297	-0.174	1.974
0021eth	H_4C_2	ethene	1.27	1.37	-0.80	0.168	1.499	-0.729	0.111
0022pro	H_6C_3	propene	1.27	1.17	-0.82	0.210	1.373	-0.723	0.139
0023str	H_6C_4	s-trans-1,3-butadiene	0.61	0.94	-1.33	-0.136	1.150	-1.207	-0.241
0024met	H_8C_4	2-methylpropene	1.16	1.34	-0.88	-0.009	1.616	-0.757	-0.120
0025buta	H_8C_4	1-butene	1.38	1.20	-0.81	0.403	1.447	-0.697	0.332
0026cyc	H_8C_5	cyclopentene	0.56	0.53	-0.63	0.253	0.800	-0.517	0.168
0027pen	$H_{10}C_5$	1-pentene	1.66	1.38	-0.85	0.633	1.679	-0.720	0.562
0028Epe	$H_{10}C_5$	E-2-pentene	1.34	1.43	-0.70	0.639	1.689	-0.607	0.543
0029hex	$H_{12}C_6$	1-hexene	1.68	1.60	-0.92	0.990	1.945	-0.763	0.921
0030eth	H_2C_2	ethyne	-0.01	-0.22	-2.21	-1.155	-0.095	-2.087	-1.267
0031pro	H_4C_3	propyne	-0.31	-0.52	-2.14	-1.258	-0.267	-1.954	-1.391
0032but	H_6C_4	1-butyne	-0.16	-0.24	-2.06	-0.807	0.065	-1.854	-0.948
0033pen	H_8C_5	1-pentyne	0.01	-0.02	-1.97	-0.513	0.312	-1.763	-0.654
0034hex	$H_{10}C_6$	1-hexyne	0.29	-0.03	-2.17	-0.287	0.379	-1.928	-0.423
0035ben	H_6C_6	benzene	-0.87	-0.71	-1.65	-1.146	-0.627	-1.592	-1.309
0036tol	H_8C_7	toluene	-0.89	-0.35	-1.64	-1.054	-0.200	-1.566	-1.249
0037eth	$H_{10}C_8$	ethylbenzene	-0.80	-0.14	-1.66	-0.788	0.078	-1.551	-0.980
0038oxy	$H_{10}C_8$	o-xylene	-0.90	-0.26	-1.71	-1.027	-0.024	-1.603	-1.236
0039mxy	$H_{10}C_8$	m-xylene	-0.84	0.05	-1.61	-0.931	0.244	-1.529	-1.158
0040pxy	$H_{10}C_8$	p-xylene	-0.81	0.10	-1.58	-0.877	0.278	-1.514	-1.096
0041nap	H_8C_{10}	naphthalene	-2.39	-1.47	-2.30	-1.980	-1.363	-2.236	-2.233
0042ant	$H_{10}C_{14}$	anthracene	-4.23	-2.20	-2.94	-2.608	-2.073	-2.863	-2.934
0044met	H_4CO	methanol	-5.11	-4.15	-3.22	-5.738	-4.184	-3.119	-6.158
0045eth	H_6C_2O	ethanol	-5.01	-4.17	-3.06	-5.578	-4.130	-2.933	-4.804
0046eth	$H_6C_2O_2$	1,2-ethanediol	-9.30	-8.70	-5.15	-8.161	-8.787	-5.009	-8.721
0047pro	H_8C_3O	1-propanol	-4.83	-4.06	-3.09	-5.133	-3.977	-2.940	-5.583
0048pro	H_8C_3O	isopropanol	-4.76	-4.26	-3.11	-4.707	-4.132	-2.959	-5.124
0049but	$H_{10}C_4O$	1-butanol	-4.72	-3.89	-3.12	-4.922	-3.773	-2.965	-5.370
0050met	$H_{10}C_4O$	t-butanol	-4.51	-3.81	-3.03	-4.444	-3.604	-2.844	-4.864
0051cyc	$H_{10}C_5O$	cyclopentanol	-5.49	-4.76	-3.03	-4.180	-4.629	-2.874	-4.600
0052pen	$H_{12}C_5O$	1-pentanol	-4.47	-3.99	-3.26	-4.460	-3.829	-3.095	-4.893
0053phe	H_6C_6O	phenol	-6.62	-5.21	-3.95	-6.720	-5.313	-3.925	-7.251
0054hex	$H_{14}C_6O$	1-hexanol	-4.36	-3.81	-3.29	-4.295	-3.619	-3.110	-4.730
0055ocr	H_8C_7O	o-cresol	-5.87	-4.56	-3.69	-6.348	-4.658	-3.680	-6.891

0056mcr	H_8C_7O	m-cresol	-5.49	-4.82	-3.96	-6.525	-4.857	-3.911	-7.068
0057pcr	H_8C_7O	p-cresol	-6.14	-4.75	-3.88	-6.461	-4.810	-3.855	-7.018
0058hep	$H_{16}C_7O$	1-heptanol	-4.24	-3.63	-3.31	-4.111	-3.410	-3.128	-4.554
0060dim	H_6C_2O	dimethylether	-1.92	-0.59	-1.82	-3.367	-0.498	-1.745	-3.677
0061tet	H_8C_4O	tetrahydrofuran	-3.47	-2.15	-2.12	-2.877	-1.966	-1.969	-3.155
0062dio	$H_8C_4O_2$	1,4-dioxane	-5.05	-4.57	-3.22	-4.453	-4.306	-2.969	-4.758
0063die	$H_{10}C_4O$	diethylether	-1.76	-1.22	-1.93	-2.659	-0.908	-1.755	-2.917
0064met	$H_{10}C_4O$	methylpropylether	-1.66	-0.53	-1.75	-2.690	-0.304	-1.621	-3.005
0065met	$H_{10}C_4O$	methylisopropylether	-2.01	-0.63	-1.79	-2.982	-0.372	-1.646	-3.306
0066dim	$H_{10}C_4O_2$	1,2-dimethoxyethane	-4.84	-2.05	-2.69	-4.165	-1.823	-2.508	-4.564
0067but	$H_{12}C_5O$	t-butylmethylether	-2.21	-0.54	-1.83	-2.392	-0.222	-1.675	-2.688
0068ani	H_8C_7O	anisole	-2.45	-1.51	-2.66	-3.035	-1.461	-2.602	-3.389
0070eth	H_4C_2O	acetaldehyde	-3.50	-3.24	-3.74	-3.709	-2.512	-3.183	-3.589
0071proa	H_6C_3O	propanal	-3.44	-3.07	-3.57	-3.359	-2.353	-3.031	-3.260
0072but	H_8C_4O	butanal	-3.18	-3.00	-3.70	-2.881	-2.186	-3.106	-2.762
0073pen	$H_{10}C_5O$	pentanal	-3.03	-2.79	-3.64	-2.845	-1.978	-3.074	-2.745
0074ben	H_6C_7O	benzaldehyde	-4.02	-3.67	-4.10	-4.231	-3.076	-3.625	-4.240
0075pro	H_6C_3O	acetone	-3.85	-4.14	-4.18	-3.565	-3.354	-3.570	-3.454
0076but	H_8C_4O	2-butanone	-3.64	-3.84	-3.94	-3.184	-3.074	-3.367	-3.112
0077cyc	H_8C_5O	cyclopentanone	-4.68	-4.70	-4.22	-2.769	-3.848	-3.552	-2.672
0078pen	$H_{10}C_5O$	2-pentanone	-3.53	-3.68	-3.98	-2.728	-2.858	-3.391	-2.654
0079pen	$H_{10}C_5O$	3-pentanone	-3.41	-3.54	-3.68	-2.760	-2.788	-3.142	-2.723
0080hex	$H_{12}C_6O$	2-hexanone	-3.29	-3.54	-4.01	-2.645	-2.681	-3.407	-2.568
0081dim	$H_{12}C_6O$	3,3-dimethylbutanone	-2.89	-3.22	-3.74	-2.503	-2.376	-3.195	-2.485
0082hep	$H_{14}C_7O$	2-heptanone	-3.04	-3.35	-4.06	-2.416	-2.460	-3.440	-2.340
0083hep	$H_{14}C_7O$	4-heptanone	-2.93	-3.25	-3.77	-1.928	-2.388	-3.202	-1.882
0084met	H_8C_8O	acetophenone	-4.58	-4.30	-4.34	-3.971	-3.702	-3.863	-4.034
0085non	$H_{18}C_9O$	5-nonanone	-2.67	-2.94	-3.85	-1.693	-2.007	-3.253	-1.648
0086eth	$H_4C_2O_2$	acetic acid	-6.70	-5.74	-4.47	-8.155	-5.374	-4.093	-8.506
0087pro	$H_6C_3O_2$	propanoic acid	-6.47	-5.51	-4.30	-7.598	-5.149	-3.935	-7.991
0088but	$H_8C_4O_2$	butanoic acid	-6.36	-5.38	-4.35	-7.066	-4.959	-3.971	-7.444
0089pen	$H_{10}C_5O_2$	pentanoic acid	-6.16	-5.28	-4.39	-6.984	-4.821	-3.993	-7.375
0090hex	$H_{12}C_6O_2$	hexanoic acid	-6.21	-5.10	-4.42	-6.760	-4.612	-4.009	-7.151
0091met	$H_4C_2O_2$	methyl formate	-2.78	-2.18	-3.56	-4.514	-1.766	-3.167	-4.617
0092ethb	$H_6C_3O_2$	ethyl formate	-2.65	-2.37	-3.59	-3.990	-1.871	-3.155	-4.063
0093met	$H_6C_3O_2$	methyl acetate	-3.32	-2.89	-3.68	-3.907	-2.505	-3.301	-4.078
0094met	$H_8C_4O_2$	methyl propanoate	-2.93	-2.68	-3.51	-3.114	-2.277	-3.139	-3.310
0095eth	$H_8C_4O_2$	ethyl acetate	-3.10	-3.11	-3.74	-3.373	-2.637	-3.310	-3.508
0096met	$H_{10}C_5O_2$	methyl butanoate	-2.83	-2.56	-3.56	-3.027	-2.108	-3.173	-3.221
0097pro	$H_{10}C_5O_2$	propyl acetate	-2.86	-3.05	-3.77	-2.940	-2.515	-3.322	-3.058
0098met	$H_{12}C_6O_2$	methyl pentanoate	-2.57	-2.41	-3.60	-2.778	-1.924	-3.205	-2.972
0099but	$H_{12}C_6O_2$	butyl acetate	-2.55	-2.91	-3.81	-2.768	-2.341	-3.346	-2.886
0100met	$H_{14}C_7O_2$	methyl hexanoate	-2.49	-2.23	-3.64	-2.636	-1.706	-3.226	-2.833
0101pen	$H_{14}C_7O_2$	pentyl acetate	-2.45	-2.73	-3.84	-2.538	-2.132	-3.367	-2.662
0103eth	H_7C_2N	ethyl amine	-4.50	-3.75	-2.79	-4.439	-3.529	-2.763	-4.684
0104dim	H_7C_2N	dimethyl amine	-4.29	-3.24	-1.96	-5.528	-3.043	-1.932	-5.884
0105aze	H_7C_3N	azetidine	-5.56	-4.70	-2.14	-5.110	-4.503	-2.097	-5.062
0106pro	H_9C_3N	propylamine	-4.39	-3.66	-2.81	-4.241	-3.393	-2.768	-4.506
0107tri	H_9C_3N	trimethylamine	-3.23	-2.50	-1.31	-6.275	-2.260	-1.274	-6.733
0108pyr	H_9C_4N	pyrrolidine	-5.48	-5.01	-2.44	-5.118	-4.722	-2.348	-5.438
0109pip	$H_{10}C_4N_2$	piperazine	-7.40	-8.11	-3.42	-7.559	-7.748	-3.299	-7.999
0110but	$H_{11}C_4N$	butylamine	-4.29	-3.46	-2.83	-3.992	-3.171	-2.788	-4.253
0111die	$H_{11}C_4N$	diethylamine	-4.07	-3.01	-1.96	-4.373	-2.665	-1.862	-4.692
0112Nme	$H_{12}C_5N_2$	N-methylpiperazine	-7.77	-7.16	-2.82	-10.029	-6.765	-2.702	-10.624
0113pen	$H_{13}C_5N$	pentylamine	-4.10	-3.30	-2.87	-3.945	-2.976	-2.810	-4.214
0114NNd	$H_{14}C_6N_2$	N,N'-dimethylpiperazine	-7.58	-6.25	-2.19	-8.576	-5.806	-2.073	-9.122
0115dip	$H_{15}C_6N$	dipropylamine	-3.66	-2.64	-2.01	-3.781	-2.225	-1.887	-4.079
0116pyr	H_5C_5N	pyridine	-4.70	-4.22	-3.21	-4.826	-3.801	-2.965	-5.022
0117met	$H_6C_5N_2$	2-methylpyrazine	-5.57	-6.03	-3.53	-5.013	-5.414	-3.199	-5.221
0118ani	H_7C_6N	aniline	-5.49	-4.75	-4.11	-5.964	-4.768	-4.179	-6.359
0119met	H_7C_6N	2-methylpyridine	-4.63	-3.62	-2.99	-4.472	-3.156	-2.737	-4.742
0120met	H_7C_6N	3-methylpyridine	-4.77	-4.04	-3.34	-4.571	-3.527	-3.057	-4.761
0121met	H_7C_6N	4-methylpyridine	-4.94	-4.17	-3.44	-4.761	-3.625	-3.131	-4.936
0122Nme	H_9C_7N	N-methylaniline	-4.68	-3.90	-3.41	-6.121	-3.818	-3.390	-6.567
0123dim	H_9C_7N	2,4-dimethylpyridine	-4.86	-3.52	-3.20	-5.029	-2.954	-2.891	-5.308
0124dim	H_9C_7N	2,5-dimethylpyridine	-4.72	-3.38	-3.09	-4.223	-2.851	-2.814	-4.488
0125dim	H_9C_7N	2,6-dimethylpyridine	-4.60	-3.03	-2.78	-4.117	-2.552	-2.532	-4.478
0126eth	H_3C_2N	acetonitrile	-3.89	-4.01	-5.44	-4.639	-3.210	-4.889	-4.518
0127pro	H_5C_3N	propionitrile	-3.85	-3.72	-5.22	-3.809	-2.885	-4.677	-3.706
0128butb	H_7C_4N	butanonitrile	-3.64	-3.55	-5.05	-3.597	-2.689	-4.514	-3.499
0129ben	H_5C_7N	benzonitrile	-4.10	-3.38	-5.01	-3.665	-2.802	-4.645	-3.684
0130nit	$H_5C_2NO_2$	nitroethane	-3.71	-3.84	-4.99	-3.748	-3.334	-4.460	-3.810

0131nit	$H_7C_3NO_2$	1-nitropropane	-3.34	-3.74	-4.98	-3.157	-3.169	-4.424	-3.197
0132nit	$H_7C_3NO_2$	2-nitropropane	-3.14	-2.86	-4.57	-3.060	-2.403	-4.108	-3.159
0133nit	$H_9C_4NO_2$	1-nitrobutane	-3.08	-3.58	-4.99	-2.978	-2.973	-4.426	-3.024
0134nit	$H_5C_6NO_2$	nitrobenzene	-4.12	-2.30	-4.47	-3.103	-1.945	-4.071	-3.213
0135met	$H_7C_7NO_2$	2-methyl-1-nitrobenzene	-3.59	-2.23	-4.39	-2.571	-1.810	-3.964	-2.684
0136met	H_4CS	methanethiol	-1.24	-0.78	-2.09	-1.019	-0.919	-2.452	-1.125
0137ethb	H_6C_2S	ethanethiol	-1.30	-0.99	-2.10	-0.656	-1.022	-2.395	-0.706
0138pro	H_8C_3S	1-propanethiol	-1.05	-0.94	-2.16	-0.408	-0.903	-2.417	-0.510
0139thi	H_6C_6S	thiophenol	-2.55	-2.09	-2.76	-2.582	-2.197	-3.007	-2.862
0140dim	H_6C_2S	dimethylsulfide	-1.54	-0.28	-2.12	-0.613	-0.319	-2.377	-0.724
0141dim	$H_6C_2S_2$	dimethyldisulfide	-1.83	-1.14	-2.38	-1.314	-1.330	-2.771	-1.449
0142die	$H_{10}C_4S$	diethylsulfide	-1.43	-0.25	-2.04	-0.056	-0.140	-2.238	-0.172
0143dip	$H_{14}C_6S$	dipropylsulfide	-1.27	-0.12	-2.16	0.526	0.115	-2.300	0.425
0144thi	H_8C_7S	thioanisole	-2.73	-1.80	-2.85	-2.097	-1.785	-3.004	-2.350
0145pro	H_6C_3O	allylalcohol	-5.08	-3.94	-3.12	-4.966	-3.877	-2.993	-5.423
0146met	$H_8C_3O_2$	2-methoxyethanol	-6.77	-6.08	-4.29	-6.991	-6.032	-4.131	-7.589
0147met	H_9C_3NO	2-methoxyethanamine	-6.55	-5.84	-4.17	-6.256	-5.680	-4.142	-6.652
0148but	H_4C_4	butenyne	0.04	0.17	-2.10	-1.185	0.360	-1.975	-1.338
0149mor	H_9C_4NO	morpholine	-7.17	-6.46	-3.39	-7.134	-6.107	-3.178	-7.555
0150mhy	$H_6C_7O_2$	m-hydroxybenzaldehyde	-9.51	-8.13	-6.37	-9.527	-7.708	-5.930	-9.891
0151phy	$H_6C_7O_2$	p-hydroxybenzaldehyde	-10.48	-8.69	-6.80	-10.152	-8.234	-6.325	-10.484
0153flu	H_3CF	fluoromethane	-0.22	-0.11	-1.89	-1.334	0.389	-1.599	-1.491
0154dif	$H_4C_2F_2$	1,1-difluoroethane	-0.11	-1.16	-2.49	-0.788	-0.226	-1.918	-0.637
0157flu	H_5C_6F	fluorobenzene	-0.78	-0.49	-1.86	-0.608	-0.103	-1.633	-0.693
0160chl	H_3CCl	chloromethane	-0.56	-0.66	-1.84	-0.853	-0.719	-2.009	-0.974
0161dic	H_2CCl_2	dichloromethane	-1.36	-1.78	-2.20	-1.555	-2.013	-2.498	-1.722
0162tri	$HCCl_3$	chloroform	-1.07	-0.99	-1.68	-1.654	-1.255	-1.967	-1.445
0163chl	H_5C_2Cl	chloroethane	-0.63	-0.93	-1.88	-0.451	-0.873	-2.002	-0.547
0165tri	$H_3C_2Cl_3$	1,1,1-trichloroethane	-0.25	-0.73	-1.56	-0.728	-0.748	-1.689	-0.799
0166tri	$H_3C_2Cl_3$	1,1,2-trichloroethane	-1.95	-2.79	-2.64	-1.680	-3.000	-2.949	-1.742
0167chla	H_7C_3Cl	1-chloropropane	-0.27	-0.88	-1.91	-0.089	-0.750	-1.995	-0.176
0168chl	H_7C_3Cl	2-chloropropane	-0.25	-0.79	-1.92	-0.139	-0.647	-1.998	-0.218
0169chl	H_3C_2Cl	chloroethene	-0.59	0.24	-1.39	-0.640	0.255	-1.483	-0.735
0170chl	H_5C_3Cl	3-chloropropene	-0.57	-0.91	-2.11	-0.859	-0.803	-2.163	-0.966
0171Zdi	$H_2C_2Cl_2$	Z-1,2-dichloroethene	-1.17	-0.59	-1.92	-1.380	-0.718	-2.118	-1.487
0172Edi	$H_2C_2Cl_2$	E-1,2-dichloroethene	-0.76	-0.04	-1.38	-0.959	-0.056	-1.495	-1.007
0173tri	HC_2Cl_3	trichloroethene	-0.39	0.70	-1.17	-1.002	0.615	-1.303	-1.062
0174chl	H_5C_6Cl	chlorobenzene	-1.12	-0.86	-1.80	-1.282	-0.847	-1.878	-1.463
0175odi	$H_4C_6Cl_2$	1,2-dichlorobenzene	-1.36	-0.82	-1.98	-1.342	-0.911	-2.169	-1.541
0176pdi	$H_4C_6Cl_2$	1,4-dichlorobenzene	-1.01	-0.88	-1.81	-1.312	-0.886	-1.940	-1.452
0177bro	H_3CBr	bromomethane	-0.82	-0.91	-1.86	-0.922	-0.716	-1.906	-1.038
0178dib	H_2CBr_2	dibromomethane	-2.11	-2.21	-2.26	-1.857	-2.070	-2.356	-2.009
0179tri	$HCBr_3$	bromoform	-1.98	-2.08	-1.90	-2.348	-2.041	-2.045	-2.291
0180bro	H_5C_2Br	bromoethane	-0.70	-1.19	-1.94	-0.574	-0.875	-1.926	-0.671
0182bro	H_7C_3Br	1-bromopropane	-0.56	-1.15	-1.98	-0.258	-0.773	-1.933	-0.340
0183bro	H_7C_3Br	2-bromopropane	-0.48	-1.04	-1.99	-0.287	-0.632	-1.936	-0.373
0184bro	H_9C_4Br	1-bromobutane	-0.41	-1.01	-2.01	-0.071	-0.587	-1.957	-0.156
0185bro	$H_{11}C_5Br$	1-bromopentane	-0.08	-0.84	-2.04	0.116	-0.380	-1.973	0.027
0186bro	H_5C_6Br	bromobenzene	-1.46	-1.42	-1.87	-1.850	-1.254	-1.902	-2.009
0187dib	$H_4C_6Br_2$	p-dibromobenzene	-2.30	-1.93	-1.93	-2.303	-1.665	-1.963	-2.429
0197bro	CF_3Br	bromotrifluoromethane	1.79	2.20	-0.56	1.465	2.300	-0.481	1.492
0198chl	H_2CFCl	chlorofluoromethane	-0.77	-1.36	-2.34	-1.612	-1.153	-2.307	-1.784
0199chl	HCF_2Cl	chlorodifluoromethane	-0.50	-0.29	-1.86	-0.987	0.019	-1.718	-1.117
0200tet	CF_4	tetrafluoromethane	3.16	3.24	-0.38	2.745	3.493	-0.263	3.176
0201bro	HC_2F_3ClBr	1-bromo-1-chloro-2,2,2-trif	-0.13	-0.11	-2.01	-0.272	0.122	-1.926	-0.372
0202bro	H_4C_2ClBr	1-bromo-2-chloroethane	-1.95	-2.47	-2.37	-1.273	-2.333	-2.482	-1.410
0203bro	HC_2F_4Br	1-bromo-1,2,2,2-tetrafluoroeth	0.52	0.21	-2.05	0.031	0.721	-1.766	-0.045
0204tet	C_2Cl_4	tetrachloroethene	0.05	1.89	-0.75	-0.611	1.877	-0.815	-0.610
0205chl	$H_2C_2F_3Cl$	1-chloro-2,2,2-trifluoroethane	0.06	-1.06	-2.52	0.051	-0.613	-2.345	-0.064
0206tri	$C_2F_3Cl_3$	1,1,2-trichloro-1,2,2-trifluoroe	1.77	2.92	-0.70	1.043	3.029	-0.562	1.077
0207tri	$H_3C_2OF_3$	2,2,2-trifluoroethanol	-4.31	-5.34	-4.90	-5.272	-4.657	-4.388	-3.897
0209chl	$H_2C_3OF_5Cl$	1-chloro-2,2,2-trifluoroethy	0.11	-0.74	-3.02	-0.786	-0.027	-2.705	-0.966
0211tri	$H_5C_3OF_3$	1,1,1-trifluoropropan-2-ol	-4.16	-3.89	-3.60	-3.652	-3.363	-3.247	-2.301
0212hex	$H_2C_3OF_6$	1,1,1,3,3,3-hexafluoropropan-2-	-3.77	-2.46	-3.37	-2.619	-1.733	-2.995	-0.943
0213bis	$H_8C_4SCl_2$	bis(2-chloroethyl)sulfide	-3.92	-4.19	-3.91	-1.586	-4.227	-4.248	-1.748
0214tri	$H_5C_4OF_3$	2,2,2-trifluorethylvinylether	-0.12	-0.52	-2.87	-0.659	0.281	-2.421	-0.831
0215pbr	H_5C_6OBr	p-bromophenol	-7.13	-6.03	-4.28	-7.577	-6.023	-4.340	-8.111
0216amm	H_3N	ammonia	-4.29	-3.60	-3.44	-4.295	-3.673	-3.667	-4.548
0217wat	H_2O	water	-6.31	-8.03	-4.65	-7.056	-8.159	-4.549	-7.525
0218pho	H_3P	phosphine	0.60	0.94	-0.64	1.694	0.437	-1.027	1.603
0219hyd	H_2S	hydrogensulfide	-0.70	-1.33	-1.94	-1.669	-1.683	-2.502	-1.792
0220tri	$H_9C_3O_4P$	trimethylphosphate	-8.70	-5.29	-6.74	-9.235	-5.609	-6.652	-9.743

0221tri	$H_{15}C_6O_4P$	triethylphosphate	-7.80	-6.22	-6.98	-7.539	-6.228	-6.721	-7.925
0222tri	$H_{21}C_9O_4P$	tripropylphosphate	-6.10	-5.96	-7.04	-6.197	-5.782	-6.699	-6.538
0223die	$H_{10}C_4S_2$	diethyldisulfide	-1.63	-0.93	-2.20	-0.484	-0.964	-2.512	-0.586
0225pipa	$H_{11}C_5N$	piperidine	-5.11	-3.32	-1.75	-5.095	-3.040	-1.679	-5.445
0227Nme	$H_{11}C_5NO$	N-methylmorpholine	-6.34	-5.44	-2.72	-8.827	-5.050	-2.511	-9.389
0228met	H_5CN	methylamine	-4.56	-3.61	-2.70	-4.816	-3.498	-2.740	-5.097
0229hyd	H_4N_2	hydrazine	-6.26	-5.28	-4.77	-7.627	-5.260	-4.953	-7.994
0230eth	$H_8C_6N_2$	2-ethylpyrazine	-5.51	-5.43	-3.36	-4.928	-4.818	-3.053	-5.174
0233ethb	H_5C_2NO	acetamide	-9.71	-9.00	-6.92	-9.584	-8.238	-6.268	-9.677
0234ENmb	H_7C_3NO	E-N-methylacetamide	-10.00	-8.56	-6.57	-8.685	-7.609	-5.777	-8.680
0235ZNmb	H_7C_3NO	Z-N-methylacetamide	-10.00	-8.64	-6.53	-9.301	-7.871	-5.858	-9.433
0236oct	$H_{18}C_8O$	1-octanol	-4.09	-3.44	-3.34	-3.902	-3.195	-3.143	-4.343
0237oct	$H_{16}C_8O$	octanal	-2.29	-2.23	-3.72	-2.257	-1.333	-3.124	-2.171
0238met	$H_{18}C_9O_2$	methyloctanoate	-2.04	-1.89	-3.69	-2.285	-1.302	-3.262	-2.486
0239oct	$H_{16}C_8O$	2-octanone	-2.88	-3.18	-4.09	-2.244	-2.252	-3.461	-2.173
0240met	$H_8C_8O_2$	methylbenzoate	-3.91	-2.67	-3.80	-3.991	-2.455	-3.549	-4.266
0242dii	$H_{14}C_6O$	isopropylether	-0.53	-0.99	-1.93	-1.955	-0.543	-1.698	-2.199
0244tet	$H_{10}C_5O$	tetrahydropyran	-3.12	-1.98	-1.94	-2.656	-1.693	-1.749	-2.892
0245thi	H_4C_4S	thiophene	-1.42	-0.64	-1.79	-1.477	-0.600	-1.817	-1.604
0246eth	$H_{10}C_8O$	ethylphenylether	-2.22	-1.55	-2.61	-2.606	-1.412	-2.502	-2.936
0400hyd	H_2	hydrogen	2.33	1.64	-0.09	0.596	1.756	-0.053	0.596
0401amia	$H_{12}C_9N_2O$	1,1-dimethyl-3-phenylurea	-9.63	-8.48	-7.03	-9.347	-8.027	-6.626	-9.630
0402adn	$H_7C_6N_5$	9-methyladenine	-13.60	-13.61	-7.59	-11.904	-12.830	-7.186	-12.489
0403thi	$H_8C_6N_2O_2$	1-methylthymine	-10.40	-11.25	-8.78	-11.752	-9.972	-7.654	-11.922
0405hex	C_2F_6	hexafluoroethane	3.94	4.20	-0.44	3.931	4.532	-0.296	3.906
0406oct	C_3F_8	octafluoropropane	4.28	5.11	-0.53	4.779	5.529	-0.353	4.753
0407tet	$H_2C_2Cl_4$	1,1,1,2-tetrachloroethane	-1.15	-1.58	-2.15	-1.549	-1.761	-2.390	-1.664
0408hex	C_2Cl_6	hexachloroethane	-1.40	1.32	-0.97	-0.914	1.313	-1.018	-0.924
0409clb	H_9C_4Cl	2-chlorobutane	0.07	-0.54	-1.83	0.119	-0.351	-1.899	0.044
0410clp	$H_{11}C_5Cl$	1-chloropentane	0.07	-0.57	-1.98	0.286	-0.355	-2.037	0.198
0411chp	$H_{11}C_5Cl$	2-chloropentane	0.07	-0.28	-1.84	0.424	-0.036	-1.888	0.348
0412clt	H_7C_7Cl	chlorotoluene	-1.92	-2.64	-3.12	-2.012	-2.592	-3.233	-2.259
0413clt	H_7C_7Cl	o-chlorotoluene	-1.15	-0.43	-1.69	-0.943	-0.344	-1.736	-1.144
0414dcl	$H_8C_{12}Cl_2$	2,2'-dichlorobiphenyl	-2.73	-1.82	-3.15	-2.116	-1.880	-3.386	-2.459
0415dcl	$H_8C_{12}Cl_2$	2,3-dichlorobiphenyl	-2.45	-1.47	-2.86	-1.884	-1.468	-3.006	-2.187
0416dcl	$H_7C_{12}Cl_3$	2,2',3'-trichlorobiphenyl	-1.99	-1.69	-3.24	-2.089	-1.832	-3.556	-2.430
0417brp	H_5C_3Br	3-bromopropene	-0.86	-1.33	-2.32	-1.049	-1.005	-2.321	-1.197
0418bri	H_9C_4Br	1-bromo-isobutane	-0.03	-0.74	-1.88	0.018	-0.315	-1.824	-0.062
0419brt	H_7C_7Br	(bromomethyl)benzene	-2.37	-2.80	-3.14	-2.172	-2.493	-3.160	-2.408
0420pbr	H_7C_7Br	p-bromotoluene	-1.39	-1.14	-1.94	-1.672	-0.890	-1.947	-1.842
0421dfl	CF_2Cl_2	difluorodichloromethane	1.69	2.30	-0.53	1.026	2.343	-0.482	1.023
0422ftc	$CFCl_3$	fluorotrichloromethane	0.82	1.70	-0.62	0.090	1.720	-0.619	0.081
0423brt	CCl_3Br	bromotrichloromethane	-0.93	0.41	-0.83	-1.128	0.393	-0.931	-1.135
0424clp	C_2F_5Cl	chloropentaflouroethane	2.86	3.89	-0.50	2.979	4.080	-0.362	2.982
0425dbr	$H_3C_7NOBr_2$	3,5-dibromo-4-hydroxybenzoni	-9.00	-4.62	-6.22	-8.948	-4.056	-5.886	-9.289
0426dcl	$H_3C_7NCl_2$	2,6-dichlorobenzonitrile	-5.22	-3.23	-5.26	-3.807	-2.824	-5.021	-3.844
0427dcl	$H_5C_7NSCl_2$	2,6-dichlorothiobenzamide	-10.81	-8.55	-7.44	-8.914	-9.039	-8.229	-9.591
0428ami	$H_3C_6N_2O_2Cl_3$	4-amino-3,5,6-trichloropyrid	-11.96	-10.64	-8.04	-13.454	-10.667	-8.079	-14.111
0433pho	$H_7C_4O_4PCl_2$	2,2-dichloroethenyldimethylp	-6.61	-3.50	-5.84	-8.034	-3.649	-5.769	-8.405
0437pho	$H_{13}C_9O_3PS_2$	methyl3-methyl-4-thiomethoxy	-6.92	-7.34	-7.81	-11.328	-8.394	-8.848	-12.372
0438pho	$H_{13}C_{10}O_3PSCl_2$	diethyl2,4-dichloropheny	-3.86	-2.62	-4.66	-3.857	-3.084	-5.280	-4.220
0440pho	$H_{12}C_9O_4PCl$	dimethyl5-(4-chloro)bicyclo	-7.28	-4.49	-5.82	-7.443	-4.574	-5.756	-7.953
0441pho	$H_{10}C_8NO_5PS$	dimethyl4-nitrophenylthiop	-7.62	-4.14	-7.55	-6.957	-4.466	-7.802	-7.442
0442pho	$H_{15}C_{11}O_3PSClBr$	O-ethylO'-4-bromo-2-c	-4.09	-6.80	-7.30	-7.697	-6.386	-7.156	-7.866
0444pho	$H_8C_8O_3PSCl_3$	dimethyl2,4,5-trichlorophe	-5.06	-2.06	-4.89	-5.048	-2.728	-5.619	-5.521
0445pho	$H_8C_8O_3PSCl_2Br$	dimethyl4-bromo-2,5-dic	-5.70	-2.46	-4.91	-5.444	-3.054	-5.620	-5.918
0447pho	$H_{14}C_{10}NO_5PS$	diethyl4-nitrophenylthiop	-6.27	-4.43	-7.21	-5.372	-4.520	-7.326	-5.684
0449pho	$H_{14}C_{15}NO_2PS$	ethyl4-cyanophenylphenylt	-5.10	-5.67	-8.14	-5.970	-5.545	-8.285	-6.264
0471dim	H_9C_7N	3,4-dimethylpyridine	-5.22	-4.26	-3.65	-4.717	-3.618	-3.284	-4.880
0506nit	H_3CNO_2	nitromethane	-3.95	-3.73	-5.16	-4.951	-3.363	-4.712	-5.063
0571dim	H_9C_7N	3,5-dimethylpyridine	-4.84	-3.82	-3.45	-4.347	-3.241	-3.137	-4.536
0574eth	H_9C_7N	4-ethylpyridine	-4.74	-4.13	-3.48	-4.644	-3.538	-3.148	-4.808
0939tet	$H_{12}C_4Si$	tetramethylsilane	3.04	3.78	-0.61	1.409	4.157	-0.431	1.368
c000	H_4O_2	waterdimer	-11.27	-13.41	-7.90	-13.055	-13.986	-7.930	-13.886
n005	H_6CN_2	methylhydrazine	-5.31	-5.08	-4.19	-8.578	-5.017	-4.326	-9.037
n006	$H_8C_2N_2$	1,1-dimethylhydrazine	-4.48	-4.67	-3.38	-9.382	-4.479	-3.434	-9.965
n007	H_4CN_2O	urea	-13.80	-12.10	-8.50	-12.703	-11.512	-7.987	-12.912
n008	H_7C_7NO	benzamide	-10.90	-8.88	-6.84	-9.613	-8.345	-6.385	-9.854
n009	H_9C_7N	2-methylaniline	-5.56	-4.34	-3.91	-5.728	-4.309	-3.979	-6.139
n010	H_9C_7N	3-methylaniline	-5.67	-4.31	-4.03	-5.805	-4.291	-4.107	-6.231
n011	H_9C_7N	4-methylaniline	-5.55	-4.19	-3.97	-5.704	-4.197	-4.069	-6.135
n013	$H_{11}C_8N$	N-ethylaniline	-4.62	-3.52	-3.36	-5.788	-3.352	-3.298	-6.214

n014	$H_{11}C_8N$	N,N-dimethylaniline	-3.58	-2.28	-2.79	-3.519	-2.077	-2.689	-3.831
n015	$H_8C_6N_2$	3,aminoaniline	-9.92	-8.70	-6.52	-9.421	-8.856	-6.763	-9.984
n016	$H_8C_2N_2$	1,2-ethanediamine	-9.72	-9.10	-5.31	-7.029	-8.840	-5.326	-7.415
n017	H_2O_2	hydrogenperoxide	-8.58	-8.95	-4.72	-8.430	-9.141	-4.701	-8.968
n018	H_4CO_2	methylperoxide	-5.28	-5.52	-3.71	-6.913	-5.610	-3.646	-7.436
n019	$H_6C_2O_2$	ethylperoxide	-5.32	-5.64	-3.73	-6.608	-5.673	-3.630	-7.154
n191	$H_4C_4N_2O_2$	uracil	-16.59	-13.60	-10.15	-14.255	-12.430	-9.069	-14.357
n200	$H_3C_4N_2O_2F$	5-fluorouracil	-16.92	-13.47	-10.63	-13.859	-11.883	-9.282	-13.811
n201	$H_3C_5N_2O_2F_3$	5-trifluoromethyluracil	-15.46	-13.00	-11.13	-12.895	-11.308	-9.764	-12.884
n202	$H_3C_4N_2O_2Cl$	5-chlorouracil	-17.74	-13.60	-10.45	-14.174	-12.544	-9.564	-14.308
n203	$H_3C_4N_2O_2Br$	5-bromouracil	-18.17	-13.62	-10.47	-14.733	-12.412	-9.526	-14.845
test0001	$H_{14}C_9O_6$	1,3-diacetyloxypropan-2-ylacetat	-8.84	-9.97	-8.31	-8.433	-9.173	-7.479	-8.794
test0004	$H_4C_8F_6$	m-bis(trifluoromethyl)benzene	1.07	0.94	-2.65	2.370	2.039	-2.071	2.269
test0005	$H_{13}C_{10}NO_2$	N,N-dimethyl-p-methoxybenzami	-11.01	-7.35	-6.95	-7.665	-6.624	-6.334	-7.911
test0006	$H_{13}C_{10}NO$	N,N,4-trimethylbenzamide	-9.76	-6.23	-5.91	-6.105	-5.396	-5.273	-6.248
test0007	$H_8C_4OCl_2$	bis(2-chloroethyl)ether	-4.23	-3.82	-3.28	-3.168	-3.702	-3.390	-3.470
test0008	$H_{10}C_6O_4$	1,1-diacetoxyethane	-4.97	-5.61	-5.84	-5.488	-4.941	-5.208	-5.684
test0009	$H_{14}C_6O_2$	1,1-diethoxyethane	-3.28	-1.85	-2.40	-3.106	-1.544	-2.174	-3.484
test0011	$H_{12}C_7O_4$	diethylpropanedioate	-6.00	-5.97	-6.09	-5.381	-5.330	-5.472	-5.603
test0012	$H_8C_3O_2$	dimethoxymethane	-2.93	-1.79	-2.51	-3.820	-1.665	-2.359	-4.174
test0013	$H_{10}C_6O_4$	ethyleneglycoldiacetate	-6.34	-5.98	-5.33	-6.335	-5.577	-4.869	-6.628
test0014	$H_{14}C_6O_2$	1,2-diethoxyethane	-3.54	-2.15	-2.56	-3.719	-1.767	-2.304	-4.120
test0016	$H_6C_7O_2$	phenylformate	-3.82	-2.84	-4.12	-4.635	-2.452	-3.763	-4.773
test0017	$H_4C_3N_2$	imidazole	-9.81	-9.04	-6.74	-11.211	-8.615	-6.480	-11.574
test1001	$H_4C_2N_2O_6$	nitroglycol	-5.70	-1.18	-6.31	-3.185	-0.621	-5.653	-3.249
test1002	$H_6C_3N_2O_6$	1,2-dinitroxypropane	-5.00	-1.71	-6.73	-3.553	-1.071	-6.053	-3.538
test1003	$H_9C_4NO_3$	butyl nitrate	-2.10	-0.10	-3.83	-1.101	0.294	-3.433	-1.133
test1004	$H_9C_4NO_3$	2-butyl nitrate	-1.80	0.00	-3.55	-1.090	0.425	-3.168	-1.084
test1005	$H_9C_4NO_3$	isobutyl nitrate	-1.90	0.09	-3.67	-1.055	0.493	-3.291	-1.076
test1006	$H_5C_2NO_4$	ethylene glycol mononitrate	-8.20	-4.92	-5.72	-6.583	-4.681	-5.308	-6.975
test1007	$H_{20}C_{14}NO_2Cl$	2-chloro-N-(2,6-diethylphe	-8.20	-5.20	-5.45	-5.646	-4.636	-5.168	-6.128
test1008	$H_{14}C_7N_2O_2S$	2-methyl-2-(methylthio)propa	-9.80	-6.82	-6.82	-7.892	-6.147	-6.442	-8.019
test1009	$H_{17}C_9N_5S$	2-(ethylamino)-4-isopropylamin	-7.70	-8.50	-5.80	-9.737	-8.175	-5.883	-10.428
test1010	$H_{12}C_{10}N_3O_3PS_2$	O,O-dimethylS-[(4-oxo-1,2	-10.00	-11.58	-9.68	-9.262	-11.857	-10.179	-9.897
test1011	$H_{16}C_{13}N_3O_4F_3$	N-butyl-N-ethyl-2,6-dinitro	-3.50	-0.84	-6.29	-0.490	0.564	-5.327	-0.649
test1012	$H_{18}C_{16}N_4O_7S$	a-[(4,6-dimethoxypyrimidin-	-17.20	-26.56	-19.46	-25.102	-26.207	-18.991	-26.262
test1013	$H_{13}C_9N_2O_2Br$	5-bromo-3-sec-butyl-6-methy	-9.70	-9.55	-8.54	-10.547	-8.615	-7.907	-10.760
test1014	$H_8C_9NO_2SCl_3$	3a,4,7,7a-tetrahydro-2-[(t	-9.00	-7.57	-7.15	-6.164	-6.789	-6.621	-6.275
test1015	$H_{11}C_{12}NO_2$	1-naphthylmethylcarbamate(car	-9.50	-8.85	-7.62	-8.930	-8.308	-7.110	-9.224
test1016	$H_{15}C_{12}NO_3$	2,3-dihydro-2,2-dimethyl-7-be	-9.60	-9.46	-8.77	-9.183	-8.823	-8.151	-9.466
test1017	$H_{16}C_{11}O_2PS_3Cl$	S-4-chlorophenylthiometh	-6.50	-2.73	-4.80	-5.502	-3.195	-5.441	-5.958
test1018	$H_6C_{10}Cl_8$	octachloro-4,7-methanohydroinda	-3.40	-3.87	-4.38	-2.037	-3.954	-4.670	-2.151
test1019	$H_{14}C_{12}O_4PCl_3$	phosphoricacid[(E)-2-chlor	-7.10	-5.62	-7.08	-7.458	-5.474	-6.956	-7.811
test1020	$H_{15}C_{15}N_4O_6SCl$	ethyl2-(4-chloro-6-metho	-14.00	-18.37	-13.84	-18.042	-18.183	-13.569	-18.827
test1021	CNO_2Cl_3	trichloro(nitro)methane(chloro	-1.50	1.77	-2.38	-1.494	1.905	-2.158	-1.422
test1022	$H_{11}C_9NO_3PSCl_3$	O,O-diethylO-3,5,6-tric	-5.00	-1.84	-4.75	-5.265	-2.417	-5.425	-5.672
test1023	$H_{17}C_{14}NO_4PS_2Cl$	S-(RS)-2-chloro-1-phth	-5.70	-9.08	-8.65	-7.941	-9.227	-8.971	-8.440
test1024	$H_{21}C_{12}N_2O_3PS$	diethoxy-[(2-isopropyl-6-	-6.50	-6.97	-6.65	-6.669	-6.985	-7.024	-7.295
test1025	$H_6C_8O_3Cl_2$	3,6-dichloro-2-methoxybenzoica	-9.90	-5.38	-5.14	-9.479	-5.455	-5.151	-10.064
test1027	$H_{13}C_{11}N_4O_4F_3$	N1,N1-diethyl-2,6-dinitro-4	-5.70	-3.67	-7.30	-4.416	-2.451	-6.418	-4.795
test1028	$H_{12}C_{10}N_2O_5$	(RS)-2-sec-butyl-4,6-dinitrop	-6.20	-8.45	-10.07	-10.371	-7.671	-9.203	-10.704
test1029	$H_6C_9O_3SCl_6$	6,7,8,9,10,10-hexachloro-1,5	-4.20	-8.77	-6.83	-8.412	-8.822	-6.816	-8.743
test1030	$H_8C_{12}OCl_6$	(1R,4S,4aS,5S,6S,7R,8R,8aR)-1	-5.50	-4.43	-4.29	-3.937	-4.342	-4.345	-4.091
test1031	$H_{22}C_9O_4P_2S_4$	O,O,O',O'-tetraethylS,S'-met	-6.10	-7.23	-8.16	-7.703	-7.927	-9.083	-8.332
test1033	$H_5C_{10}Cl_7$	1,4,5,6,7,8,8-heptachloro-3a,4,	-2.60	-1.97	-3.22	-1.861	-1.966	-3.426	-1.992
test1034	$H_{14}C_9O$	3,5,5-trimethyl-2-cyclohexen-1-o	-5.20	-5.20	-5.32	-3.540	-4.055	-4.505	-3.396
test1035	$H_6C_6Cl_6$	1,2,3,4,5,6-hexachlorocyclohexan	-5.40	-6.40	-4.90	-3.073	-6.609	-5.292	-3.245
test1036	$H_{19}C_{10}O_6PS_2$	2-(dimethoxyphosphinothioyl	-8.20	-6.51	-8.03	-9.511	-6.753	-8.197	-10.095
test1037	$H_{10}C_5N_2O_2S$	N-methylcarbamic acid[1-(meth	-10.70	-8.07	-7.56	-10.632	-7.462	-7.111	-10.858
test1039	$H_{15}C_{14}N_5O_6S$	methyl2-(4-methoxy-6-methyl	-15.50	-22.01	-15.74	-19.028	-21.659	-15.340	-19.899
test1040	$H_{19}C_{13}N_3O_6S$	4-mesyl-2,6-dinitro-N,N-dip	-8.00	-10.42	-11.52	-8.455	-9.627	-10.726	-8.958
test1041	$H_5C_3NO_4$	nitroxyacetone	-6.00	-3.93	-5.89	-4.069	-3.068	-5.128	-4.077
test1043	$H_{14}C_{10}NO_5PS$	O,O-diethyl-O-4-nitro-phe	-6.70	-5.02	-7.78	-5.794	-5.110	-7.887	-6.148
test1044	$H_{21}C_{10}NOS$	S-propylbutyl(ethyl)thiocar	-3.60	-3.12	-4.24	-3.228	-2.265	-3.853	-3.311
test1045	$H_{17}C_7O_2PS_3$	O,O-diethylS-ethylthiomethyl	-4.40	-4.52	-5.67	-4.846	-4.971	-6.425	-5.204
test1046	$H_{16}C_{14}N_3O_4F_3$	N-cyclopropylmethyl-2,6-din	-2.50	-2.17	-6.56	-0.644	-0.876	-5.650	-0.837
test1047	$H_{19}C_{10}N_5S$	N2,N4-diisopropyl-6-methylthi	-8.40	-8.30	-5.80	-9.238	-7.894	-5.866	-9.939
test1048	$H_9C_9NOCl_2$	N-(3,4-dichlorophenyl)propan	-7.80	-7.03	-6.27	-9.288	-6.661	-6.078	-9.516
test1049	$H_8C_{10}N_3OCl$	5-amino-4-chloro-2-phenyl-3	-16.40	-11.66	-9.43	-11.486	-11.276	-9.186	-11.891
test1050	$H_{12}C_7N_5Cl$	6-chloro-N,N'-diethyl-1,3,5-t	-10.20	-11.61	-6.31	-9.387	-11.206	-6.289	-10.020
test1051	$H_{16}C_{15}N_4O_5S$	methyl2-(4,6-dimethylpyrimi	-20.30	-21.20	-15.74	-19.821	-20.646	-15.247	-20.686
test1052	$H_{13}C_9N_2O_2Cl$	3-t-butyl-5-chloro-6-methyl	-11.10	-8.78	-7.78	-9.579	-8.083	-7.304	-9.881

test1053	$H_{19}C_{10}N_5S$	N2-tert-butyl-N4-ethyl-6-meth	-6.70	-7.93	-5.59	-9.328	-7.563	-5.662	-10.021
test1054	$H_{13}C_{12}N_5O_6S_2$	3-(4-methoxy-6-methyl-1,3,5	-16.20	-23.20	-17.03	-20.394	-22.622	-16.460	-21.190
test1055	$H_8C_4O_4PCl_3$	dimethyl(RS)-2,2,2-trichloro	-12.70	-8.33	-7.66	-13.285	-8.830	-7.785	-14.055
test1056	$H_{16}C_{13}N_3O_4F_3$	a,a,a-trifluoro-2,6-dinitro	-3.30	-1.35	-6.46	-0.542	0.000	-5.509	-0.714
test1057	$H_{21}C_{10}NOS$	S-propyldipropyl(thiocarbam	-4.10	-3.32	-4.10	-2.799	-2.476	-3.738	-2.899
test1058	$H_{10}C_{12}N_4O_2$	4-amino-4'-nitroazobenzene	-11.20	-8.86	-8.52	-9.908	-8.449	-8.164	-10.414
test1059	$H_{14}C_{20}N_2O_2$	1-amino-4-anilinoanthraquinon	-7.40	-8.39	-6.85	-8.290	-7.933	-6.498	-8.838
test1060	$H_{12}C_{14}N_4O_2$	1,4,5,8-tetraminoanthraquinon	-8.90	-13.03	-9.15	-13.201	-13.149	-9.296	-14.012
test1061	$H_9C_{14}NO_2$	1-amino-anthraquinone	-8.00	-7.47	-6.21	-7.290	-6.972	-5.788	-7.565
test1063	$H_{18}C_{11}N_4O_2$	(2-dimethylamino-5,6-dimethyl	-9.40	-7.67	-6.95	-9.206	-6.978	-6.473	-9.693
test2001	$H_8C_9O_4$	acetylsalicylic acid	-9.94	-7.59	-6.59	-10.730	-7.338	-6.202	-11.285
test2003	$H_{14}C_{11}O_3$	butylparaben	-8.72	-7.46	-6.47	-8.623	-7.253	-6.168	-9.177
test2004	$H_{10}C_8N_4O_2$	caffeine	-12.64	-11.57	-8.40	-9.667	-10.597	-7.561	-10.130
test2006	$H_3C_4N_2O_2Cl$	6-chlorouracil	-15.83	-11.10	-8.51	-12.867	-10.043	-7.504	-12.891
test2007	$H_3C_3N_3O_3$	cyanuric acid	-18.06	-14.38	-10.30	-15.327	-13.061	-9.109	-15.534
test2010	$H_8C_{13}O_3F_2$	diflunisal	-9.40	-12.14	-9.33	-12.678	-11.642	-8.806	-13.322
test2011	$H_{10}C_9O_3$	ethylparaben	-9.20	-7.68	-6.38	-9.260	-7.559	-6.110	-9.828
test2013	$H_{13}C_{15}O_2F$	flurbiprofen(racemic)	-8.42	-6.83	-6.16	-8.699	-6.175	-5.699	-9.329
test2015	C_6Cl_6	hexachlorobenzene	-2.33	1.42	-1.56	-0.783	1.495	-1.604	-0.773
test2017	$H_{18}C_{13}O_2$	ibuprofen(racemic)	-7.00	-5.10	-5.06	-7.712	-4.578	-4.690	-8.290
test2018	$H_3C_4N_2O_2I$	5-iodouracil	-18.72	-14.77	-10.40	-15.070	-13.937	-9.633	-15.276
test2019	$H_{14}C_{16}O_3$	ketoprofen(racemic)	-10.78	-9.70	-7.71	-10.386	-9.135	-7.194	-10.985
test2020	$H_8C_8O_3$	methylparaben	-9.51	-7.44	-6.31	-9.851	-7.402	-6.090	-10.466
test2021	$H_{14}C_{14}O_3$	naproxen	-10.21	-7.79	-6.73	-10.438	-7.525	-6.444	-11.206
test2022	$H_6C_6N_2O_2$	4-nitroaniline	-9.45	-8.13	-8.20	-8.755	-7.772	-7.790	-9.017
test2023	C_4F_8	octafluorocyclobutane	3.43	3.28	-1.40	4.372	4.135	-1.019	4.312
test2024	$C_6NO_2Cl_5$	pentachloronitrobenzene	-5.22	2.04	-3.36	-2.231	2.253	-3.080	-2.132
test2025	$H_5C_8NO_2$	phthalimide	-9.61	-8.28	-6.82	-9.627	-7.375	-6.015	-9.656
test2026	$H_{12}C_{10}O_3$	propylparaben	-9.37	-7.62	-6.41	-8.832	-7.443	-6.123	-9.383
test2027	$H_8C_4O_2S$	sulfolane	-8.61	-11.36	-8.02	-8.108	-11.291	-7.848	-8.639
test2029	$H_9C_5O_3F_3$	trimethylorthotrifluoroacetate	-0.80	0.24	-3.02	-1.947	0.415	-2.837	-2.374
test3001	$H_9C_8NO_2$	paracetamol	-14.83	-12.14	-8.63	-12.995	-11.770	-8.183	-13.547
test3002	$H_9C_8NO_2$	N-(3-hydroxyphenyl)acetamide	-13.93	-11.83	-8.58	-12.839	-11.491	-8.158	-13.231
test3003	$H_{14}C_{16}O_3$	fenbufen	-12.75	-14.30	-10.70	-13.922	-13.592	-10.002	-14.475
test3004	$H_9C_8NO_2$	N-(2-hydroxyphenyl)acetamide	-11.61	-9.98	-7.39	-11.637	-9.680	-7.029	-12.181
test3005	$H_{13}C_{10}NO_2$	phenacetin	-10.91	-8.50	-7.33	-10.554	-7.889	-6.794	-10.890
test3007	$H_8C_8O_3$	2-methoxybenzoic acid	-10.32	-7.20	-6.11	-10.323	-7.218	-5.914	-10.934
test3014	$H_8C_8O_3$	4-methoxybenzoic acid	-9.15	-6.43	-5.69	-9.753	-6.250	-5.409	-10.296
test3015	$H_8C_8O_3$	3-methoxybenzoic acid	-8.93	-6.28	-5.62	-9.687	-6.138	-5.375	-10.263
test3019	$H_{12}C_{14}NO_2Cl$	tolfenamic acid	-6.71	-4.89	-4.58	-8.226	-4.766	-4.532	-8.943
test3020	$H_{11}C_{14}NO_2Cl_2$	diclofenac	-6.30	-10.38	-9.19	-11.391	-10.162	-8.936	-11.855
test3021	$H_{10}C_{14}NO_2F_3$	flufenamic acid	-5.68	-9.94	-9.81	-9.525	-9.114	-9.132	-9.910
test4001	H_5C_6I	iodobenzene	-1.73	-1.67	-1.90	-2.341	-1.805	-1.995	-2.493
test4002	H_2CI_2	diiodomethane	-2.49	-3.53	-2.22	-2.386	-4.090	-2.420	-2.428
test4003	H_3CI	iodomethane	-0.89	-0.92	-1.69	-1.087	-1.101	-1.774	-1.116
test4004	H_5C_2I	iodoethane	-0.72	-1.06	-1.76	-0.746	-1.145	-1.821	-0.772
test4006	H_7C_3I	1-iodopropane	-0.59	-0.97	-1.80	-0.464	-0.983	-1.830	-0.490
test4007	H_9C_4I	1-iodobutane	-0.25	-0.81	-1.84	-0.304	-0.782	-1.854	-0.335
test4008	$H_{11}C_5I$	1-iodopentane	-0.12	-0.68	-1.85	-0.043	-0.621	-1.860	-0.072
test4009	H_7C_3I	2-iodopropane	-0.46	-0.87	-1.81	-0.460	-0.879	-1.869	-0.484

Subsets of neutral molecules:

Small molecules:
0001met, 0030eth, 0153flu, 0160chl, 0161dic, 0162tri, 0177bro, 0178dib, 0179tri, 0197bro, 0198chl, 0199chl, 0200tet, 0216amm, 0217wat, 0218pho, 0219hyd, 0400hyd, 0421dfl, 0422ftc, 0423brt, n017, test4002, test4003

Alcohols:
0044met, 0045eth, 0046eth, 0047pro, 0048pro, 0049but, 0050met, 0051cyc, 0052pen, 0053phe, 0054hex, 0055ocr, 0056mcr, 0057pcr, 0058hep, 0145pro, 0146met, 0236oct

Aldehydes and ketones:
0070eth, 0071proa, 0072but, 0073pen, 0074ben, 0145pro, 0150mhy, 0151phy, 0237oct, test2001, 0075pro, 0076but, 0077cyc, 0078pen, 0079pen, 0080hex, 0081dim, 0082hep, 0083hep, 0084met, 0085non, 0239oct

Ethers:
0060dim, 0063die, 0064met, 0065met, 0067but, 0242dii, 0246eth, 0062dio, 0068ani, 0061tet

Esters:
0091met, 0092ethb, 0093met, 0094met, 0095eth, 0096met, 0097pro, 0098met, 0099but, 0100met, 0101pen, 0238met, 0240met, test0011, test0013, test0016, test2003, test2011, test2020, test2026, test0013

Acids:
test2021, 0086eth, 0087pro, 0088but, 0089pen, 0090hex, test2001, test3007, test3014, test3015

Amines:
0103eth, 0104dim, 0105aze, 0106pro, 0107tri, 0108pyr, 0109pip, 0110but, 0111die, 0112Nme, 0113pen, 0114NNd, 0115dip, 0116pyr, 0117met, 0118ani, 0119met, 0120met, 0121met, 0122Nme, 0123dim, 0124dim, 0125dim, 0216amm, 0225pipa, 0228met, 0229hyd, 0230eth, 0402adn, 0471dim, 0571dim, 0574eth, n005, n006, n009, n010, n011, n013, n014, n015, n016, test0017

Nitriles:
0126eth, 0127pro, 0128butb, 0129ben

Nitro compounds and nitrates:
0130nit, 0131nit, 0132nit, 0133nit, 0134nit, 0135met, 0506nit, test1001, test1002, test1028, test1041, test1058, test2022, test1003, test1004, test1005, test1006

Fluorine compounds:
0153flu, 0154dif, 0157flu, 0197bro, 0198chl, 0199chl, 0200tet, 0201bro, 0203bro, 0205chl, 0206tri, 0207tri, 0209chl, 0211tri, 0212hex, 0214tri, 0405hex, 0406oct, 0421dfl, 0422ftc, 0424clp, n200, n201, test0004, test1011, test1027, test1046, test1056, test2010, test2013, test2023, test2029, test3021

Chlorine compounds:
0160chl, 0161dic, 0162tri, 0163chl, 0165tri, 0166tri, 0167chla, 0168chl, 0169chl, 0170chl, 0171Zdi, 0172Edi, 0173tri, 0174chl, 0175odi, 0176pdi, 0198chl, 0199chl, 0201bro, 0202bro, 0204tet, 0205chl, 0206tri, 0209chl, 0213bis, 0407tet, 0408hex, 0409clb, 0410clp, 0411chp, 0412clt, 0413clt, 0414dcl, 0415dcl, 0416dcl, 0421dfl, 0422ftc, 0423brt, 0424clp, 0426dcl, 0427dcl, 0428ami, 0433pho, 0438pho, 0440pho, 0442pho, 0444pho, 0445pho, n202, test0007, test1007, test1014, test1017, test1018, test1019, test1020, test1021, test1022, test1023, test1025, test1029, test1030, test1033, test1035, test1048, test1049, test1050, test1052, test1055, test2006, test2015, test2024, test3019, test3020

Bromine compounds:
0177bro, 0178dib, 0179tri, 0180bro, 0182bro, 0183bro, 0184bro, 0185bro, 0186bro, 0187dib, 0197bro, 0201bro, 0202bro, 0203bro, 0215pbr, 0417brp, 0418bri, 0419brt, 0420pbr, 0423brt, 0425dbr, 0442pho, 0445pho, n203, test1013

Iodine compounds:
0939tet, test2018, test4001, test4002, test4003, test4004, test4006, test4007, test4008, test4009

Training set for neutral molecules:

0017cyc, 0019met, 0036tol, 0037eth, 0038oxy, 0039mxy, 0040pxy, 0048pro, 0050met, 0052pen, 0053phe, 0054hex, 0058hep, 0067but, 0071proa, 0094met, 0097pro, 0100met, 0101pen, 0103eth, 0106pro, 0109pip, 0113pen, 0115dip, 0116pyr, 0119met, 0121met, 0123dim, 0127pro, 0128butb, 0130nit, 0131nit, 0132nit, 0133nit, 0139thi, 0145pro, 0149mor, 0150mhy, 0157flu, 0163chl, 0167chla, 0168chl, 0169chl, 0174chl, 0175odi, 0177bro, 0180bro, 0187dib, 0201bro, 0205chl, 0216amm, 0222tri, 0225pipa, 0233ethb, 0237oct, 0240met, 0245thi, 0405hex, 0409clb, 0412clt, 0416dcl, 0418bri, 0424clp, 0425dbr, 0438pho, 0440pho, 0444pho, 0574eth, n009, n010, n011, n014, n017, test0009, test0013, test0014, test1021, test1024, test1037, test2003, test2011, test2025, test3004, test3007, test4002, test4004, test4006, test4007, test4008, test4009

Table S4. Mean signed error (MSE), mean absolute error (MAE), and standard deviation (SD) of the hydration free energy in kcal/mol for 143 ions calculated by our method, SMD, and PCM methods with respect to the reference values.

Dataset		Solvation scheme		
		xESE	SMD[a]	PCM[a]
All ions(143)[b]	MSE	-0.87	6.14	12.18
	MAE	3.00	6.28	12.18
	SD	4.29	7.58	13.51
All cations(60)	MSE	-0.17	3.44	12.28
	MAE	2.91	3.76	12.28
	SD	3.83	5.08	13.35
Small cations(8)[d]	MSE	-4.05	7.17	18.44
	MAE	5.49	7.17	18.44
	SD	6.92	8.42	19.88
Oxygen-containing cations(21)	MSE	1.96	6.69	16.76
	MAE	3.22	6.84	16.76
	SD	3.59	7.73	17.78
Halogen-containing cations(2)	MSE	1.08	4.10	13.70
	MAE	1.08	4.10	13.70
	SD	1.40	4.12	13.71
All anions(83)	MSE	-1.38	8.09	12.10
	MAE	3.06	8.10	12.10
	SD	4.59	8.97	13.62
Small anions(37)[d]	MSE	-3.39	7.08	9.80
	MAE	4.07	7.08	9.80
	SD	5.89	8.19	11.98
Oxygen-containing anions(68)	MSE	-1.01	7.95	13.62
	MAE	2.91	7.97	13.62
	SD	4.16	8.87	14.73
Halogen-containing anions(16)	MSE	-2.73	7.47	7.81
	MAE	3.03	7.47	7.81
	SD	4.73	8.28	9.50
Linear correlation[c] (for all 143 ions)				
	Slope	0.98	0.78	0.58
	Intercept	–2.01	–9.81	–17.93
	R	0.927	0.908	0.849

[a] Calculated using the Gaussian program package.
[b] The complete list of ions see Tables S1 and S2.
[c] Linear correlation between ΔG°_{solv} obtained within a given method and $\Delta^{ref}G^{\circ}_{solv}$.
[d] Less than 6 atoms.

Table S5. Mean signed error (MSE), mean absolute error (MAE), and standard deviation (SD) of the hydration free energy in kcal·mol^{-1} for 390 neutral molecules calculated by our method, SMD, and PCM methods with respect to the reference values $\Delta^{ref}G^{\circ}_{solv}$.

Dataset	Solvation scheme		
	xESE	SMD[a]	PCM[a]

All molecules(390)[b]	MSE	-0.05	0.57	0.31
	MAE	0.90	1.15	1.85
	SD	1.38	1.70	2.34
Small molecules(24)[c]	MSE	-0.41	–0.05	–0.89
	MAE	0.55	0.46	1.45
	SD	0.72	0.63	1.75
Alcohols(18)	MSE	0.02	0.82	1.88
	MAE	0.38	0.82	1.88
	SD	0.55	0.86	2.03
Aldehydes and ketones(22)	MSE	0.40	0.27	0.12
	MAE	0.51	0.49	1.05
	SD	0.66	0.77	1.47
Ethers(10)	MSE	-0.57	0.90	0.16
	MAE	0.81	0.99	0.61
	SD	0.90	1.07	0.87
Esters(21)	MSE	-0.25	0.53	0.07
	MAE	0.37	0.61	1.20
	SD	0.58	0.85	1.49
Acids(10)	MSE	-0.70	1.82	2.78
	MAE	0.70	1.82	2.78
	SD	0.81	2.01	2.90
Amines(42)	MSE	-0.30	0.81	2.16
	MAE	0.80	0.87	2.16
	SD	1.31	0.95	2.48
Nitriles(4)	MSE	-0.06	0.22	–1.31
	MAE	0.32	0.27	1.31
	SD	0.43	0.37	1.33
Nitro compounds and nitrates(17)				
	MSE	0.55	1.36	–0.81
	MAE	1.16	1.74	1.57
	SD	1.53	2.10	1.80
Fluorine compounds(33)				
	MSE	0.22	0.31	–1.78
	MAE	1.19	1.08	2.62
	SD	1.62	1.49	2.98
Chlorine compounds(74)				
	MSE	0.10	0.82	0.03
	MAE	1.06	1.68	1.73
	SD	1.62	2.28	2.35
Bromine compounds(25)				
	MSE	-0.05	0.30	–0.34
	MAE	0.53	0.97	1.61
	SD	1.05	1.60	2.22
Iodine compounds(10)				
	MSE	0.14	0.14	–0.30
	MAE	0.65	0.81	2.01
	SD	1.28	1.35	3.05
All molecules(390)	MSE	-0.30	0.87	0.50
6-31G* basis set[d]	MAE	0.99	1.34	1.91
	SD	1.50	1.87	2.47
Linear correlation[f] (for all 390 molecules)				
	Slope	0.95	0.92	0.57
	Intercept	–0.29	0.23	–1.58
	R	0.952	0.934	0.883

[a] Calculated using the Gaussian program package.
[b] The complete list of ions see Table S3.
[c] Less than six atoms.
[d] For iodine, the LANL2DZ pseudopotential and corresponding basis set were used.
[f] Linear correlation between ΔG°_{solv} obtained within a given method and $\Delta^{ref}G^{\circ}_{solv}$.

Table S6. **Pomogaeva–Chipman subset – cations – solvation energy in kcal/mol**

Code	Exper.	CMIRS	xESE	SMD	PCM
i088	-110.3	-121.63	-110.293	-96.2	-77.6
i015	-50.9	-45.91	-45.201	-52.9	-46.3
i028	-54.0	-47.89	-51.861	-53.5	-46.3
i027	-55.9	-52.04	-55.340	-54.9	-48.4
i037	-56.0	-54.26	-56.782	-54.2	-47.9
i026	-57.2	-53.88	-57.598	-56.9	-49.7
i011	-60.5	-56.50	-58.968	-60.5	-52.8
i035	-61.4	-61.80	-67.284	-62.7	-54.9

i012	-61.6	-55.93	-60.821	-60.3	-52.9
i024	-62.6	-61.00	-63.513	-62.2	-53.8
i034	-63.3	-59.39	-60.990	-61.9	-53.2
i033	-64.2	-60.91	-64.086	-63.1	-54.7
i023	-65.8	-69.38	-70.619	-67.3	-57.2
i099	-67.2	-66.84	-65.071	-62.3	-52.7
i006	-67.3	-64.31	-68.051	-66.3	-57.4
i029	-67.4	-67.42	-66.625	-65.5	-55.6
i009	-68.6	-66.12	-73.398	-67.7	-60.1
i007	-68.7	-64.90	-66.906	-66.2	-56.9
i021	-69.8	-68.04	-69.169	-65.9	-57.1
i019	-70.3	-67.13	-68.480	-66.6	-57.0
i030	-70.9	-69.69	-76.891	-70.5	-61.2
i018	-72.4	-70.17	-72.688	-68.1	-58.8
i098	-73.9	-74.56	-76.849	-70.3	-60.2
i126	-74.1	-73.50	-73.912	-70.4	-60.8
i125	-74.7	-73.31	-72.734	-70.2	-60.6
i040	-75.3	-78.72	-80.086	-65.9	-60.0
i094	-75.9	-82.50	-80.113	-77.5	-68.5
i003	-76.4	-74.52	-83.922	-74.4	-65.7
i052	-79.7	-79.98	-77.523	-69.3	-60.0
i048	-84.6	-82.49	-90.936	-80.1	-69.9
i047	-85.2	-85.34	-100.248	-82.3	-72.7
i051	-88.4	-89.82	-82.475	-75.9	-63.1
i050	-93.0	-96.86	-91.315	-80.5	-67.3
i014	-54.6	-49.36	-50.296	-55.8	-49.0
i036	-61.1	-60.82	-65.799	-59.6	-53.2
i013	-61.1	-59.35	-61.480	-62.0	-55.4
i025	-62.2	-57.29	-59.520	-60.1	-51.6
i010	-63.4	-58.59	-63.399	-62.8	-54.9
i056	-64.5	-55.99	-60.103	-56.9	-48.5
i106	-64.5	-57.85	-67.177	-59.2	-57.3
i039	-66.0	-62.94	-67.372	-67.0	-55.7
i032	-66.0	-62.69	-66.927	-64.5	-56.4
i031	-67.7	-60.93	-70.593	-66.5	-58.4
i112	-67.7	-66.42	-68.415	-60.8	-55.9
i020	-69.6	-68.20	-69.145	-65.9	-57.2
i005	-69.6	-67.29	-72.028	-68.7	-59.9
i095	-69.6	-66.95	-70.526	-69.3	-58.8
i093	-71.2	-68.53	-68.886	-65.6	-56.9
i053	-71.5	-65.22	-65.698	-62.7	-53.7
i004	-71.5	-69.63	-74.262	-70.0	-61.2
i008	-72.0	-69.58	-74.457	-69.8	-61.2
i054	-77.1	-71.27	-74.110	-67.5	-57.9

Table S7. **Pomogaeva–Chipman subset – anions – solvation energy in kcal/mol**

Code	Exper.	CMIRS	xESE	SMD	PCM
i114	-104.4	-115.11	-116.076	-91.2	-87.6
i089	-104.7	-109.55	-104.697	-101.8	-85.7
i117	-54.1	-52.81	-61.905	-49.1	-52.9
i104	-57.4	-55.93	-58.999	-50.3	-49.4
i102	-57.8	-57.15	-58.390	-49.6	-48.9
i118	-59.3	-64.93	-66.555	-58.3	-57.3
i100	-60.1	-64.35	-61.630	-55.1	-53.3
i101	-61.9	-62.65	-60.706	-51.7	-50.7
i120	-62.3	-62.96	-68.741	-60.1	-57.0
i044	-62.9	-67.48	-69.653	-57.9	-56.4
i123	-66.1	-67.32	-66.699	-56.7	-54.5
i041	-66.6	-69.16	-66.605	-61.2	-62.3
i116	-68.3	-62.54	-68.305	-53.9	-67.3
i063	-68.5	-70.91	-71.978	-64.9	-60.7
i119	-69.7	-67.85	-72.685	-64.5	-60.4
i109	-70.5	-60.28	-68.415	-58.0	-65.1
i076	-71.1	-71.58	-69.626	-60.3	-56.7
i108	-71.8	-60.50	-70.765	-58.7	-65.5
i074	-71.9	-71.64	-70.705	-60.9	-57.1
i043	-72.2	-73.58	-71.317	-64.6	-65.4
i086	-73.7	-70.78	-73.213	-61.5	-57.3
i062	-74.0	-74.36	-76.234	-67.9	-63.2
i115	-74.5	-68.79	-74.481	-67.3	-72.9

i121	-77.5	-80.08	-77.761	-66.6	-61.5
i105	-80.2	-73.74	-79.002	-68.7	-63.7
i091	-83.3	-85.12	-86.578	-83.2	-73.3
i069	-84.2	-80.93	-80.621	-69.5	-61.7
i072	-85.1	-81.01	-76.964	-67.8	-60.5
i078	-85.3	-91.89	-89.287	-80.7	-69.5
i068	-86.3	-84.61	-84.271	-72.7	-64.4
i071	-86.6	-85.95	-84.692	-73.1	-65.4
i067	-88.3	-88.31	-85.590	-74.6	-66.1
i083	-89.2	-88.36	-89.661	-82.3	-71.0
i073	-89.4	-88.49	-86.161	-75.4	-66.8
i066	-90.7	-88.64	-88.777	-75.5	-67.0
i082	-93.2	-88.82	-92.759	-83.1	-71.9
i065	-95.0	-93.45	-95.229	-79.5	-70.7
i090	-97.3	-94.05	-90.294	-93.0	-78.4
i045	-54.6	-54.72	-59.301	-48.1	-47.8
i110	-63.4	-55.48	-62.399	-52.7	-57.1
i122	-65.5	-70.64	-65.696	-57.4	-55.5
i124	-66.0	-66.28	-65.646	-55.9	-53.0
i112	-67.7	-71.09	-68.415	-60.8	-55.9
i075	-70.2	-69.65	-68.853	-59.1	-55.4
i046	-70.2	-73.82	-72.841	-65.1	-67.8
i064	-71.2	-72.06	-69.619	-64.5	-59.8
i077	-72.0	-72.05	-69.431	-60.3	-56.6
i111	-72.1	-64.17	-72.087	-65.0	-71.0
i080	-73.8	-72.27	-72.527	-63.7	-57.9
i107	-73.8	-62.79	-74.280	-61.1	-68.2
i061	-74.6	-73.36	-73.209	-67.9	-62.7
i085	-76.2	-75.79	-79.643	-66.1	-62.2
i058	-76.2	-75.26	-83.744	-70.6	-66.0
i060	-76.2	-74.34	-76.894	-69.4	-63.6
i084	-76.5	-77.17	-83.159	-67.1	-63.6
i001	-76.5	-73.53	-93.557	-71.4	-70.3
i103	-76.5	-72.43	-83.976	-65.9	-63.3
i081	-77.6	-75.46	-73.737	-66.1	-59.3
i059	-77.6	-75.89	-80.307	-71.1	-65.2
i070	-82.3	-81.55	-80.987	-70.7	-62.4

Table S8.**Pomogaeva–Chipman subset – neutrals – solvation energy in kcal/mol**

Code	Exper.	CMIRS	xESE	SMD	PCM
0030eth	-0.01	-0.85	-1.155	-0.22	-2.21
0418bri	-0.03	-1.34	0.018	-0.74	-1.88
0185bro	-0.08	-1.37	0.116	-0.84	-2.04
0154dif	-0.11	-1.34	-0.788	-1.16	-2.49
0201bro	-0.13	-2.14	-0.272	-0.11	-2.01
0032but	-0.16	-0.73	-0.807	-0.24	-2.06
0153flu	-0.22	-0.52	-1.334	-0.11	-1.89
0167chla	-0.27	-0.89	-0.089	-0.88	-1.91
0031pro	-0.31	-0.68	-1.258	-0.52	-2.14
0173tri	-0.39	-0.84	-1.002	0.70	-1.17
0184bro	-0.41	-1.20	-0.071	-1.01	-2.01
0183bro	-0.48	-1.23	-0.287	-1.04	-1.99
0199chl	-0.50	-1.10	-0.987	-0.29	-1.86
0242dii	-0.53	-2.65	-1.955	-0.99	-1.93
0170chl	-0.57	-1.36	-0.859	-0.91	-2.11
0163chl	-0.63	-0.77	-0.451	-0.93	-1.88
0172Edi	-0.76	-0.58	-0.959	-0.04	-1.38
0198chl	-0.77	-1.41	-1.612	-1.36	-2.34
0157flu	-0.78	-2.06	-0.608	-0.49	-1.86
0040pxy	-0.81	-1.28	-0.877	0.10	-1.58
0177bro	-0.82	-0.62	-0.922	-0.91	-1.86
0039mxy	-0.84	-1.20	-0.931	0.05	-1.61
0417brp	-0.86	-1.54	-1.049	-1.33	-2.32
0035ben	-0.87	-1.48	-1.146	-0.71	-1.65
0038oxy	-0.90	-1.54	-1.027	-0.26	-1.71
0423brt	-0.93	-0.96	-1.128	0.41	-0.83
0176pdi	-1.01	-2.14	-1.312	-0.88	-1.81
0138pro	-1.05	-1.14	-0.408	-0.94	-2.16
0162tri	-1.07	-1.53	-1.654	-0.99	-1.68
0174chl	-1.12	-1.95	-1.282	-0.86	-1.80

0171Zdi	-1.17	-1.42	-1.380	-0.59	-1.92
0136met	-1.24	-0.81	-1.019	-0.78	-2.09
0143dip	-1.27	-1.36	0.526	-0.12	-2.16
0137ethb	-1.30	-1.02	-0.656	-0.99	-2.10
0420pbr	-1.39	-2.27	-1.672	-1.14	-1.94
0408hex	-1.40	-1.76	-0.914	1.32	-0.97
0245thi	-1.42	-1.89	-1.477	-0.64	-1.79
0142die	-1.43	-1.13	-0.056	-0.25	-2.04
0186bro	-1.46	-2.24	-1.850	-1.42	-1.87
0140dim	-1.54	-1.11	-0.613	-0.28	-2.12
0223die	-1.63	-1.68	-0.484	-0.93	-2.20
0064met	-1.66	-2.08	-2.690	-0.53	-1.75
0063die	-1.76	-2.61	-2.659	-1.22	-1.93
0141dim	-1.83	-1.79	-1.314	-1.14	-2.38
0179tri	-1.98	-2.13	-2.348	-2.08	-1.90
0416dcl	-1.99	-3.27	-2.089	-1.69	-3.24
0403thi	-10.40	-12.29	-11.752	-11.25	-8.78
0151phy	-10.48	-12.14	-10.152	-8.69	-6.80
0427dcl	-10.81	-10.05	-8.914	-8.55	-7.44
n008	-10.90	-10.38	-9.613	-8.88	-6.84
c000	-11.27	-12.33	-13.055	-13.41	-7.90
0428ami	-11.96	-13.01	-13.454	-10.64	-8.04
0402adn	-13.60	-10.40	-11.904	-13.61	-7.59
n007	-13.80	-11.02	-12.703	-12.10	-8.50
0065met	-2.01	-2.33	-2.982	-0.63	-1.79
0178dib	-2.11	-1.83	-1.857	-2.21	-2.26
0067but	-2.21	-2.72	-2.392	-0.54	-1.83
0246eth	-2.22	-3.30	-2.606	-1.55	-2.61
0237oct	-2.29	-4.47	-2.257	-2.23	-3.72
0187dib	-2.30	-2.45	-2.303	-1.93	-1.93
0419brt	-2.37	-3.33	-2.172	-2.80	-3.14
0041nap	-2.39	-2.98	-1.980	-1.47	-2.30
0098met	-2.57	-4.14	-2.778	-2.41	-3.60
0092ethb	-2.65	-3.70	-3.990	-2.37	-3.59
0085non	-2.67	-4.88	-1.693	-2.94	-3.85
0091met	-2.78	-3.60	-4.514	-2.18	-3.56
0096met	-2.83	-3.98	-3.027	-2.56	-3.56
0097pro	-2.86	-4.12	-2.940	-3.05	-3.77
0239oct	-2.88	-5.15	-2.244	-3.18	-4.09
0081dim	-2.89	-4.85	-2.503	-3.22	-3.74
0073pen	-3.03	-4.01	-2.845	-2.79	-3.64
0082hep	-3.04	-4.89	-2.416	-3.35	-4.06
0133nit	-3.08	-4.72	-2.978	-3.58	-4.99
0095eth	-3.10	-3.99	-3.373	-3.11	-3.74
0244tet	-3.12	-3.64	-2.656	-1.98	-1.94
0132nit	-3.14	-4.51	-3.060	-2.86	-4.57
0072but	-3.18	-3.97	-2.881	-3.00	-3.70
0107tri	-3.23	-1.80	-6.275	-2.50	-1.31
0080hex	-3.29	-4.72	-2.645	-3.54	-4.01
0093met	-3.32	-4.00	-3.907	-2.89	-3.68
0131nit	-3.34	-4.64	-3.157	-3.74	-4.98
0079pen	-3.41	-4.21	-2.760	-3.54	-3.68
0071proa	-3.44	-3.83	-3.359	-3.07	-3.57
0061tet	-3.47	-3.73	-2.877	-2.15	-2.12
0078pen	-3.53	-4.61	-2.728	-3.68	-3.98
n014	-3.58	-2.97	-3.519	-2.28	-2.79
0135met	-3.59	-5.52	-2.571	-2.23	-4.39
0115dip	-3.66	-2.93	-3.781	-2.64	-2.01
0130nit	-3.71	-4.64	-3.748	-3.84	-4.99
0212hex	-3.77	-6.01	-2.619	-2.46	-3.37
0438pho	-3.86	-4.39	-3.857	-2.62	-4.66
0126eth	-3.89	-5.12	-4.639	-4.01	-5.44
0240met	-3.91	-5.47	-3.991	-2.67	-3.80
0213bis	-3.92	-3.62	-1.586	-4.19	-3.91
0506nit	-3.95	-4.56	-4.951	-3.73	-5.16
0074ben	-4.02	-6.02	-4.231	-3.67	-4.10
0111die	-4.07	-3.09	-4.373	-3.01	-1.96
0134nit	-4.12	-5.58	-3.103	-2.30	-4.47
0211tri	-4.16	-5.44	-3.652	-3.89	-3.60
0058hep	-4.24	-5.83	-4.111	-3.63	-3.31
0207tri	-4.31	-7.62	-5.272	-5.34	-4.90
0054hex	-4.36	-5.65	-4.295	-3.81	-3.29

0106pro	-4.39	-4.58	-4.241	-3.66	-2.81
0052pen	-4.47	-5.52	-4.460	-3.99	-3.26
n006	-4.48	-4.61	-9.382	-4.67	-3.38
0103eth	-4.50	-4.37	-4.439	-3.75	-2.79
0050met	-4.51	-5.07	-4.444	-3.81	-3.03
0228met	-4.56	-3.98	-4.816	-3.61	-2.70
0084met	-4.58	-6.50	-3.971	-4.30	-4.34
0125dim	-4.60	-4.13	-4.117	-3.03	-2.78
n013	-4.62	-4.04	-5.788	-3.52	-3.36
0119met	-4.63	-4.70	-4.472	-3.62	-2.99
0116pyr	-4.70	-5.17	-4.826	-4.22	-3.21
0574eth	-4.74	-5.58	-4.644	-4.13	-3.48
0048pro	-4.76	-5.04	-4.707	-4.26	-3.11
0120met	-4.77	-5.31	-4.571	-4.04	-3.34
0047pro	-4.83	-5.15	-5.133	-4.06	-3.09
0123dim	-4.86	-4.86	-5.029	-3.52	-3.20
0121met	-4.94	-5.46	-4.761	-4.17	-3.44
0045eth	-5.01	-4.96	-5.578	-4.17	-3.06
0062dio	-5.05	-4.61	-4.453	-4.57	-3.22
0145pro	-5.08	-5.04	-4.966	-3.94	-3.12
n018	-5.28	-5.58	-6.913	-5.52	-3.71
n005	-5.31	-5.26	-8.578	-5.08	-4.19
n019	-5.32	-5.77	-6.608	-5.64	-3.73
0108pyr	-5.48	-4.58	-5.118	-5.01	-2.44
0230eth	-5.51	-4.18	-4.928	-5.43	-3.36
n011	-5.55	-5.73	-5.704	-4.19	-3.97
0117met	-5.57	-4.50	-5.013	-6.03	-3.53
n010	-5.67	-5.67	-5.805	-4.31	-4.03
0055ocr	-5.87	-6.56	-6.348	-4.56	-3.69
0057pcr	-6.14	-6.98	-6.461	-4.75	-3.88
0089pen	-6.16	-7.12	-6.984	-5.28	-4.39
0090hex	-6.21	-7.39	-6.760	-5.10	-4.42
0229hyd	-6.26	-5.38	-7.627	-5.28	-4.77
0217wat	-6.31	-7.22	-7.056	-8.03	-4.65
0088but	-6.36	-7.06	-7.066	-5.38	-4.35
0087pro	-6.47	-7.01	-7.598	-5.51	-4.30
0147met	-6.55	-5.85	-6.256	-5.84	-4.17
0433pho	-6.61	-5.48	-8.034	-3.50	-5.84
0053phe	-6.62	-7.12	-6.720	-5.21	-3.95
0146met	-6.77	-6.47	-6.991	-6.08	-4.29
0215pbr	-7.13	-7.94	-7.577	-6.03	-4.28
0149mor	-7.17	-5.20	-7.134	-6.46	-3.39
0114NNd	-7.58	-2.89	-8.576	-6.25	-2.19
0441pho	-7.62	-8.39	-6.957	-4.14	-7.55
0112Nme	-7.77	-4.25	-10.029	-7.16	-2.82
n017	-8.58	-7.12	-8.430	-8.95	-4.72
0220tri	-8.70	-7.71	-9.235	-5.29	-6.74
0046eth	-9.30	-9.08	-8.161	-8.70	-5.15
0401amia	-9.63	-9.57	-9.347	-8.48	-7.03
0233ethb	-9.71	-9.48	-9.584	-9.00	-6.92
n016	-9.72	-7.20	-7.029	-9.10	-5.31
n015	-9.92	-8.80	-9.421	-8.70	-6.52
0033pen	0.01	-0.88	-0.513	-0.02	-1.97
0148but	0.04	-1.01	-1.185	0.17	-2.10
0204tet	0.05	-0.50	-0.611	1.89	-0.75
0205chl	0.06	-1.91	0.051	-1.06	-2.52
0209chl	0.11	-3.19	-0.786	-0.74	-3.02
0034hex	0.29	-1.05	-0.287	-0.03	-2.17
0203bro	0.52	-1.95	0.031	0.21	-2.05
0026cyc	0.56	0.00	0.253	0.53	-0.63
0218pho	0.60	1.03	1.694	0.94	-0.64
0023str	0.61	-0.01	-0.136	0.94	-1.33
0016cyc	0.75	0.55	0.516	0.07	-0.62
0422ftc	0.82	-0.06	0.090	1.70	-0.62
0024met	1.16	0.40	-0.009	1.34	-0.88
0017cyc	1.20	0.50	1.196	1.26	-0.18
0018cyc	1.23	0.25	1.583	1.35	-0.15
0028Epe	1.34	0.71	0.639	1.43	-0.70
0025buta	1.38	0.36	0.403	1.20	-0.81
0020cis	1.58	0.10	1.998	1.97	-0.25
0027pen	1.66	0.27	0.633	1.38	-0.85
0029hex	1.68	0.37	0.990	1.60	-0.92

0421dfl	1.69	0.38	1.026	2.30	-0.53
0019met	1.71	0.24	1.711	1.75	-0.20
0206tri	1.77	-0.65	1.043	2.92	-0.70
0197bro	1.79	0.34	1.465	2.20	-0.56
0002eth	1.83	1.75	0.873	1.79	-0.11
0003pro	1.96	1.40	1.097	1.83	-0.15
0001met	2.00	2.03	0.674	2.20	-0.12
0004nbu	2.08	1.24	1.262	2.01	-0.18
0010met	2.32	1.01	1.263	2.05	-0.20
0006nhe	2.49	1.04	1.647	2.36	-0.23
0011dim	2.50	0.59	1.468	2.25	-0.30
0012met	2.52	0.89	1.724	2.38	-0.25
0007nhe	2.62	0.88	1.850	2.54	-0.26
0014tri	2.85	0.53	2.109	2.73	-0.38
0424clp	2.86	0.16	2.979	3.89	-0.50
0013dim	2.88	0.81	1.930	2.65	-0.31
0008noc	2.89	0.64	0.139	2.71	-0.29
0939tet	3.04	1.16	1.409	3.78	-0.61
0200tet	3.16	1.01	2.745	3.24	-0.38
0405hex	3.94	0.54	3.931	4.20	-0.44
0406oct	4.28	0.02	4.779	5.11	-0.53
0214tri	-0.12	-2.59	-0.659	-0.52	-2.87
0165tri	-0.25	-1.42	-0.728	-0.73	-1.56
0168chl	-0.25	-1.07	-0.139	-0.79	-1.92
0182bro	-0.56	-1.08	-0.258	-1.15	-1.98
0160chl	-0.56	-0.49	-0.853	-0.66	-1.84
0169chl	-0.59	-0.28	-0.640	0.24	-1.39
0180bro	-0.70	-0.92	-0.574	-1.19	-1.94
0219hyd	-0.70	-0.38	-1.669	-1.33	-1.94
0037eth	-0.80	-1.24	-0.788	-0.14	-1.66
0036tol	-0.89	-1.39	-1.054	-0.35	-1.64
0407tet	-1.15	-2.41	-1.549	-1.58	-2.15
0413clt	-1.15	-1.84	-0.943	-0.43	-1.69
0175odi	-1.36	-2.44	-1.342	-0.82	-1.98
0161dic	-1.36	-1.55	-1.555	-1.78	-2.20
0412clt	-1.92	-3.16	-2.012	-2.64	-3.12
0060dim	-1.92	-2.13	-3.367	-0.59	-1.82
0166tri	-1.95	-2.54	-1.680	-2.79	-2.64
0202bro	-1.95	-1.80	-1.273	-2.47	-2.37
0234ENmb	-10.00	-9.17	-8.685	-8.56	-6.57
0235ZNmb	-10.00	-8.96	-9.301	-8.64	-6.53
0415dcl	-2.45	-3.77	-1.884	-1.47	-2.86
0068ani	-2.45	-3.57	-3.035	-1.51	-2.66
0101pen	-2.45	-4.43	-2.538	-2.73	-3.84
0100met	-2.49	-4.34	-2.636	-2.23	-3.64
0099but	-2.55	-4.32	-2.768	-2.91	-3.81
0139thi	-2.55	-2.94	-2.582	-2.09	-2.76
0414dcl	-2.73	-3.16	-2.116	-1.82	-3.15
0144thi	-2.73	-3.14	-2.097	-1.80	-2.85
0083hep	-2.93	-4.38	-1.928	-3.25	-3.77
0094met	-2.93	-3.85	-3.114	-2.68	-3.51
0070eth	-3.50	-3.71	-3.709	-3.24	-3.74
0076but	-3.64	-4.58	-3.184	-3.84	-3.94
128butb	-3.64	-5.06	-3.597	-3.55	-5.05
0075pro	-3.85	-4.67	-3.565	-4.14	-4.18
0127pro	-3.85	-4.98	-3.809	-3.72	-5.22
0236oct	-4.09	-6.01	-3.902	-3.44	-3.34
0129ben	-4.10	-6.15	-3.665	-3.38	-5.01
0113pen	-4.10	-4.78	-3.945	-3.30	-2.87
0042ant	-4.23	-4.57	-2.608	-2.20	-2.94
0216amm	-4.29	-5.12	-4.295	-3.60	-3.44
0110but	-4.29	-4.66	-3.992	-3.46	-2.83
0104dim	-4.29	-2.89	-5.528	-3.24	-1.96
0122Nme	-4.68	-4.42	-6.121	-3.90	-3.41
0077cyc	-4.68	-5.46	-2.769	-4.70	-4.22
0049but	-4.72	-5.24	-4.922	-3.89	-3.12
0124dim	-4.72	-4.82	-4.223	-3.38	-3.09
0066dim	-4.84	-2.81	-4.165	-2.05	-2.69
0571dim	-4.84	-5.39	-4.347	-3.82	-3.45
0044met	-5.11	-5.07	-5.738	-4.15	-3.22
0225pipa	-5.11	-3.48	-5.095	-3.32	-1.75
0426dcl	-5.22	-6.58	-3.807	-3.23	-5.26

0471dim	-5.22	-5.85	-4.717	-4.26	-3.65
0118ani	-5.49	-5.82	-5.964	-4.75	-4.11
0051cyc	-5.49	-5.60	-4.180	-4.76	-3.03
0056mcr	-5.49	-6.99	-6.525	-4.82	-3.96
n009	-5.56	-5.47	-5.728	-4.34	-3.91
0105aze	-5.56	-2.39	-5.110	-4.70	-2.14
0227Nme	-6.34	-4.11	-8.827	-5.44	-2.72
0086eth	-6.70	-7.07	-8.155	-5.74	-4.47
0109pip	-7.40	-5.08	-7.559	-8.11	-3.42
0425dbr	-9.00	-8.53	-8.948	-4.62	-6.22
0150mhy	-9.51	-11.13	-9.527	-8.13	-6.37
0410clp	0.07	-1.12	0.286	-0.57	-1.98
0409clb	0.07	-1.21	0.119	-0.54	-1.83
0411chp	0.07	-0.95	0.424	-0.28	-1.84
0021eth	1.27	0.97	0.168	1.37	-0.80
0022pro	1.27	0.71	0.210	1.17	-0.82
0400hyd	2.33	2.37	0.596	1.64	-0.09
0005npe	2.33	1.16	1.477	2.18	-0.21

Table S9. Calculated (B3LYP/Def2TZVP) and experimental gas-phase deprotonation energies (in kcal/mol), solvation energies of selected weak acids $\Delta G^{o}_{solv}(HX)$ and corresponding anions $\Delta G^{o}_{solv}(X^{-})$ and calculated and experimental pK_a values.

	$HX \rightarrow X^{-} + H^{+}$ ΔG^{o} gas phase, kcal/mol		**$\Delta G^{o}_{solv}(X^{-})$, kcal/mol**			**ΔG^{o}_{solv} (HX) , kcal/mol**			**pK_a**			
Acid HX	**B3LYP**	**ref.**	**xESE**	**SMD**	**PCM**	**xESE**	**SMD**	**PCM**	**xESE**	**SMD**	**PCM**	**ref.**
acetic	341.252	340.7[a], 341.5[b]	-80.152	-71.078	-65.180	-7.984	-5.790	-4.477	3.72	8.77	12.13	4.76[(d)]
propionic	339.955	340.4[b]	-76.882	-69.247	-63.509	-7.586	-5.496	-4.329	4.88	8.94	12.29	4.88[(d)]
butyric	340.349	339.5[b]	-74.753	-68.470	-62.910	-6.940	-5.416	-4.361	6.25	9.74	13.04	4.82[(f)]
nitrous	336.196	330.1[a]	-74.984	-68.972	-66.085	-6.898	-2.035	-2.767	3.01	3.85	6.50	3.35[(h)]
phenol	342.172	342.3[a]	-70.658	-60.951	-57.144	-6.705	-5.274	-3.984	10.42	16.49	18.33	9.99[(j)]
MSE									**0.10**	**-4.00**	**-6.90**	
MAE									**0.65**	**4.00**	**6.90**	
SD									**0.83**	**4.46**	**7.16**	

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