PART I. Composition of the training and test sets

Table S-1. Composition of the training [(a)] and test [(b)] sets. Experimental hydration free energies[1-7] (kcal/mol) and corresponding values calculated with PW, GF methods as well as the SDC model based on these methods (kcal/mol). PLHNC closure, Lorentz-Berthelot mixing rules.

Name	ρV	N_{br}	N_{db}	N_{bz}	N_{OH}	N_{ph}	N_{Hal}	N_{eth}	N_{ald}	N_{ket}	$\Delta\mu_{hyd}^{PW}$	$\Delta\mu_{hyd}^{GF}$	$\Delta\mu_{hyd}^{SDC+PW}$	$\Delta\mu_{hyd}^{SDC+GF}$	$\Delta\mu_{hyd}^{\exp}$	
alkane																
2,2,4-trimethylpentane	4.86	3	0	0	0	0	0	0	0	0	9.79	-0.65	2.07	1.52	2.87	[a]
2,2,5-trimethylhexane	5.39	3	0	0	0	0	0	0	0	0	10.67	-0.94	2.14	1.58	2.79	[a]
2,2-dimethylbutane	4.14	2	0	0	0	0	0	0	0	0	10.22	2.20	2.52	2.53	2.57	[a]
2,4-dimethylpentane	4.65	2	0	0	0	0	0	0	0	0	11.15	1.98	2.69	2.63	2.87	[a]
2-methylbutane	3.86	1	0	0	0	0	0	0	0	0	11.25	4.34	2.90	3.10	2.38	[a]
2-methylhexane	4.88	1	0	0	0	0	0	0	0	0	12.83	3.65	2.94	3.06	2.93	[a]
n-decane	6.57	0	0	0	0	0	0	0	0	0	16.33	3.87	2.83	2.97	3.16	[a]
n-hexane	4.54	0	0	0	0	0	0	0	0	0	13.33	5.23	2.89	3.03	2.50	[a]
n-octane	5.57	0	0	0	0	0	0	0	0	0	14.96	4.67	2.96	3.13	2.89	[a]
n-pentane	4.04	0	0	0	0	0	0	0	0	0	12.47	5.47	2.79	2.96	2.36	[a]
propane	3.00	0	0	0	0	0	0	0	0	0	10.70	5.96	2.57	2.79	1.97	[a]
2,2-dimethylpentane	4.63	2	0	0	0	0	0	0	0	0	11.07	1.73	2.63	2.38	2.88	[b]
2,3,4-trimethylpentane	4.82	3	0	0	0	0	0	0	0	0	9.56	-0.45	1.90	1.70	2.56	[b]
2,3-dimethylpentane	4.57	2	0	0	0	0	0	0	0	0	10.59	1.64	2.24	2.24	2.52	[b]
2-methylpentane	4.36	1	0	0	0	0	0	0	0	0	11.95	3.93	2.84	3.01	2.52	[b]
3-methylhexane	4.81	1	0	0	0	0	0	0	0	0	12.26	3.20	2.48	2.56	2.71	[b]
3-methylpentane	4.29	1	0	0	0	0	0	0	0	0	11.37	3.47	2.36	2.51	2.51	[b]
ethane	2.45	0	0	0	0	0	0	0	0	0	9.56	5.94	2.27	2.42	1.84	[b]
methane	1.79	0	0	0	0	0	0	0	0	0	7.66	5.11	1.37	1.17	1.98	[b]
n-butane	3.47	0	0	0	0	0	0	0	0	0	11.35	5.52	2.53	2.64	2.09	[b]
n-heptane	5.04	0	0	0	0	0	0	0	0	0	14.08	4.91	2.88	3.04	2.63	[b]
n-nonane	6.05	0	0	0	0	0	0	0	0	0	15.56	4.19	2.84	2.95	3.14	[b]
alkene																
3-methylbut-1-ene	3.81	1	1	0	0	0	0	0	0	0	11.39	4.87	2.19	2.37	1.82	[a]
but-1-ene	3.38	0	1	0	0	0	0	0	0	0	11.17	5.78	1.55	1.63	1.37	[a]
ethene	2.22	0	1	0	0	0	0	0	0	0	8.41	5.21	0.55	0.31	1.28	[a]
hept-1-ene	4.93	0	1	0	0	0	0	0	0	0	13.81	5.04	1.86	1.86	1.66	[a]

hex-1-ene	4.41	0	1	0	0	0	0	0	0	0	12.94	5.27	1.77	1.77	1.64	[a]
non-1-ene	5.95	0	1	0	0	0	0	0	0	0	15.43	4.44	1.93	1.91	2.06	[a]
2-methylbut-2-ene	3.84	1	1	0	0	0	0	0	0	0	11.90	5.69	2.66	3.21	1.31	[b]
oct-1-ene	5.45	0	1	0	0	0	0	0	0	0	14.68	4.79	1.94	1.94	2.08	[b]
pent-1-ene	3.90	0	1	0	0	0	0	0	0	0	12.11	5.58	1.71	1.74	1.66	[b]
propene	2.84	0	1	0	0	0	0	0	0	0	10.06	5.81	1.27	1.30	1.29	[b]
trans-hept-2-ene	4.98	0	1	0	0	0	0	0	0	0	14.42	5.66	2.39	2.52	1.67	[b]
alkylbenzene																
ethylbenzene	4.59	1	0	1	0	0	0	0	0	0	10.59	2.35	-0.57	-0.45	-0.73	[a]
n-butylbenzene	5.59	1	0	1	0	0	0	0	0	0	12.19	1.58	-0.47	-0.60	-0.40	[a]
n-hexylbenzene	6.60	1	0	1	0	0	0	0	0	0	13.67	0.87	-0.51	-0.67	-0.04	[a]
n-pentylbenzene	6.09	1	0	1	0	0	0	0	0	0	12.87	1.21	-0.54	-0.65	-0.23	[a]
n-propylbenzene	5.11	1	0	1	0	0	0	0	0	0	11.66	2.23	-0.28	-0.25	-0.53	[a]
toluene	4.14	1	0	1	0	0	0	0	0	0	10.06	2.94	-0.40	-0.16	-0.84	[a]
1,2,3-trimethylbenzene	4.93	3	0	1	0	0	0	0	0	0	8.49	-0.71	-1.04	-0.52	-1.21	[b]
1,2,4-trimethylbenzene	5.06	3	0	1	0	0	0	0	0	0	9.52	0.23	-0.21	0.50	-0.83	[b]
1,3,5-trimethylbenzene	5.1	3	0	1	0	0	0	0	0	0	9.77	0.33	-0.01	0.62	-0.90	[b]
2-ethyltoluene	4.92	2	0	1	0	0	0	0	0	0	9.44	0.30	-1.14	-0.91	-1.04	[b]
4-ethyltoluene	5.14	2	0	1	0	0	0	0	0	0	11.01	1.62	0.10	0.55	-0.95	[b]
isobutylbenzene	5.34	2	0	1	0	0	0	0	0	0	10.21	-0.21	-1.00	-1.16	0.16	[b]
m-xylene	4.64	2	0	1	0	0	0	0	0	0	10.13	1.85	-0.02	0.47	-0.82	[b]
o-xylene	4.53	2	0	1	0	0	0	0	0	0	9.31	1.17	-0.69	-0.29	-0.90	[b]
p-xylene	4.69	2	0	1	0	0	0	0	0	0	10.55	2.27	0.32	0.91	-0.80	[b]
sec-butylbenzene	5.35	2	0	1	0	0	0	0	0	0	10.46	0.02	-0.76	-0.92	-0.45	[b]
tert-butylbenzene	5.15	3	0	1	0	0	0	0	0	0	9.13	-1.38	-0.73	-1.06	-0.44	[b]
alcohols																
2-methylbutan-1-ol	3.85	1	0	0	1	0	0	0	0	0	2.84	-6.87	-4.75	-4.79	-4.42	[a]
3-methylbutan-1-ol	3.88	1	0	0	1	0	0	0	0	0	3.74	-6.03	-3.90	-3.94	-4.42	[a]
4-methylpentan-2-ol	4.29	2	0	0	1	0	0	0	0	0	2.86	-7.92	-4.33	-4.17	-3.74	[a]
butan-1-ol	3.54	0	0	0	1	0	0	0	0	0	3.86	-4.88	-4.33	-4.38	-4.72	[a]
butan-2-ol	3.46	1	0	0	1	0	0	0	0	0	2.62	-6.06	-4.39	-4.23	-4.60	[a]
decan-1-ol	6.60	0	0	0	1	0	0	0	0	0	8.76	-6.62	-4.07	-4.17	-3.64	[a]
ethanol	2.47	0	0	0	1	0	0	0	0	0	1.63	-4.82	-4.95	-5.00	-5.00	[a]
heptan-1-ol	5.09	0	0	0	1	0	0	0	0	0	6.50	-5.56	-4.04	-4.08	-4.23	[a]

2-methylbutan-2-ol	3.78	2	0	0	1	0	0	0	0	0	2.52	-7.15	-3.91	-3.73	-4.43	[b]
2-methylpentan-2-ol	4.28	2	0	0	1	0	0	0	0	0	3.31	-7.50	-3.87	-3.76	-3.93	[b]
2-methylpentan-3-ol	4.26	2	0	0	1	0	0	0	0	0	3.57	-7.13	-3.59	-3.40	-3.89	[b]
2-methylpropan-1-ol	3.43	1	0	0	1	0	0	0	0	0	2.88	-5.72	-4.08	-3.91	-4.51	[b]
hexan-1-ol	4.57	0	0	0	1	0	0	0	0	0	5.69	-5.27	-4.07	-4.12	-4.39	[b]
hexan-3-ol	4.48	1	0	0	1	0	0	0	0	0	4.64	-6.33	-3.91	-3.85	-4.07	[b]
methanol	1.88	0	0	0	1	0	0	0	0	0	-0.07	-5.46	-5.76	-6.02	-5.11	[b]
nonan-1-ol	6.10	0	0	0	1	0	0	0	0	0	8.02	-6.24	-4.05	-4.12	-3.89	[b]
octan-1-ol	5.60	0	0	0	1	0	0	0	0	0	7.26	-5.88	-4.05	-4.08	-4.09	[b]
pentan-1-ol	4.05	0	0	0	1	0	0	0	0	0	4.71	-5.09	-4.25	-4.28	-4.52	[b]
pentan-2-ol	3.97	1	0	0	1	0	0	0	0	0	3.51	-6.29	-4.26	-4.13	-4.39	[b]
pentan-3-ol	3.93	1	0	0	1	0	0	0	0	0	3.23	-6.65	-4.49	-4.52	-4.35	[b]
propan-1-ol	3.02	0	0	0	1	0	0	0	0	0	3.10	-4.45	-4.32	-4.28	-4.83	[b]
propan-2-ol	2.97	1	0	0	1	0	0	0	0	0	2.29	-5.25	-3.97	-3.73	-4.76	[b]
phenols																
3,5-dimethylphenol	4.63	3	0	1	1	1	0	0	0	0	4.16	-6.42	-5.70	-5.45	-6.27	[a]
3-ethylphenol	4.59	2	0	1	1	1	0	0	0	0	4.45	-6.05	-6.42	-6.49	-6.26	[a]
4-ethylphenol	4.61	2	0	1	1	1	0	0	0	0	4.59	-5.91	-6.30	-6.34	-6.14	[a]
p-cresol	4.15	2	0	1	1	1	0	0	0	0	4.12	-5.29	-6.09	-6.01	-6.14	[a]
phenol	3.61	1	0	1	1	1	0	0	0	0	3.53	-4.68	-6.92	-7.13	-6.61	[a]
2,3-dimethylphenol	4.51	3	0	1	1	1	0	0	0	0	4.15	-6.24	-5.54	-5.34	-6.16	[b]
2,4-dimethylphenol	4.64	3	0	1	1	1	0	0	0	0	4.88	-5.62	-4.99	-4.64	-6.01	[b]
2,5-dimethylphenol	4.65	3	0	1	1	1	0	0	0	0	4.06	-6.35	-5.82	-5.37	-5.92	[b]
2,6-dimethylphenol	4.55	3	0	1	1	1	0	0	0	0	4.08	-6.24	-5.66	-5.32	-5.27	[b]
3,4-dimethylphenol	4.55	3	0	1	1	1	0	0	0	0	3.47	-6.99	-6.27	-6.07	-6.51	[b]
4-n-propylphenol	5.12	2	0	1	1	1	0	0	0	0	5.68	-6.04	-5.99	-6.14	-5.91	[b]
4-tert-butylphenol	5.15	4	0	1	1	1	0	0	0	0	3.25	-9.57	-6.33	-6.88	-5.95	[b]
o-cresol	4.12	2	0	1	1	1	0	0	0	0	4.63	-4.71	-5.53	-5.45	-5.88	[b]
chloroalkanes																
1-chlorobutane	3.93	0	0	0	0	0	1	0	0	0	11.32	4.52	-0.31	-0.45	-0.16	[a]
1-chloroheptane	5.48	0	0	0	0	0	1	0	0	0	13.92	3.80	-0.05	-0.19	0.29	[a]
1-chlorohexane	4.97	0	0	0	0	0	1	0	0	0	13.14	4.13	-0.06	-0.18	0.00	[a]
1-chloropentane	4.45	0	0	0	0	0	1	0	0	0	12.20	4.32	-0.21	-0.32	-0.07	[a]
1-chloropropane	3.42	0	0	0	0	0	1	0	0	0	10.48	4.88	-0.37	-0.42	-0.30	[a]

2-chloro-2-methylpropane	3.78	2	0	0	0	0	1	0	0	0	10.83	4.31	1.57	2.02	1.09	[a]
2-chlorobutane	3.85	1	0	0	0	0	1	0	0	0	10.98	4.38	0.54	0.74	0.00	[a]
2-chloropropane	3.37	1	0	0	0	0	1	0	0	0	10.28	4.80	0.58	0.86	-0.25	[a]
chloroethane	2.9	0	0	0	0	0	1	0	0	0	9.29	4.77	-0.78	-0.86	-0.63	[a]
chloromethane	2.35	0	0	0	0	0	1	0	0	0	7.74	4.20	-1.49	-1.78	-0.54	[a]
aldehydes																
acetaldehyde	2.37	0	0	0	0	0	0	0	1	0	4.65	0.15	-3.42	-3.50	-3.51	[a]
butyraldehyde	3.45	0	0	0	0	0	0	0	1	0	6.81	0.12	-2.90	-2.83	-3.18	[a]
formaldehyde	1.81	0	0	0	0	0	0	0	1	0	2.75	-0.88	-4.48	-4.88	-2.76	[a]
isobutyraldehyde	3.40	1	0	0	0	0	0	0	1	0	6.60	-0.02	-1.95	-1.62	-2.86	[a]
pentanal	3.97	0	0	0	0	0	0	0	1	0	7.68	-0.17	-2.81	-2.79	-3.03	[a]
propionaldehyde	2.93	0	0	0	0	0	0	0	1	0	5.71	0.14	-3.21	-3.15	-3.44	[a]
heptanal	5.00	0	0	0	0	0	0	0	1	0	9.42	-0.62	-2.64	-2.59	-2.67	[b]
hexanal	4.49	0	0	0	0	0	0	0	1	0	8.51	-0.41	-2.76	-2.71	-2.81	[b]
nonanal	6.02	0	0	0	0	0	0	0	1	0	10.96	-1.30	-2.62	-2.62	-2.07	[b]
octanal	5.52	0	0	0	0	0	0	0	1	0	10.22	-0.95	-2.61	-2.59	-2.29	[b]
ketones																
3-methylbutan-2-one'	3.79	2	0	0	0	0	0	0	0	1	6.54	-1.04	-3.07	-2.9549	-3.25	[a]
butanone	3.41	1	0	0	0	0	0	0	0	1	6.39	-0.22	-3.72	-2.95	-3.71	[a]
hexan-2-one	4.46	1	0	0	0	0	0	0	0	1	8.43	-0.43	-3.26	-3.76	-3.29	[a]
pentan-2-one	3.93	1	0	0	0	0	0	0	0	1	7.43	-0.26	-3.46	-3.31	-3.52	[a]
pentan-3-one	3.96	1	0	0	0	0	0	0	0	1	7.23	-0.44	-3.71	-3.48	-3.41	[a]
propanone	2.87	1	0	0	0	0	0	0	0	1	5.55	0.06	-3.74	-3.63	-3.81	[a]
4-methylpentan-2-one	4.28	2	0	0	0	0	0	0	0	1	7.16	-1.64	-3.19	-3.24	-3.05	[b]
decan-2-one	6.48	1	0	0	0	0	0	0	0	1	11.55	-1.75	-3.20	-3.34	-2.34	[b]
heptan-2-one	4.96	1	0	0	0	0	0	0	0	1	9.16	-0.77	-3.29	-3.34	-3.04	[b]
nonan-2-one	5.98	1	0	0	0	0	0	0	0	1	10.83	-1.36	-3.16	-3.27	-2.50	[b]
nonan-5-one	6.02	1	0	0	0	0	0	0	0	1	11.09	-1.13	-2.96	-3.02	-2.65	[b]
octan-2-one	5.48	1	0	0	0	0	0	0	0	1	9.98	-1.06	-3.24	-3.30	-2.88	[b]
undecan-2-one	6.99	1	0	0	0	0	0	0	0	1	12.26	-2.12	-3.25	-3.40	-2.16	[b]
ethers																
di-n-butyl ether	5.91	0	0	0	0	0	0	1	0	0	13.43	1.86	-0.78	-0.84	-0.83	[a]
di-n-propyl ether	4.93	0	0	0	0	0	0	1	0	0	12.26	3.06	-0.47	-0.26	-1.16	[a]
diethyl ether	3.85	0	0	0	0	0	0	1	0	0	9.38	2.36	-1.72	-1.65	-1.60	[a]

diisopropyl ether	4.56	2	0	0	0	0	0	1	0	0	9.04	-0.11	-1.00	-0.89	-0.53	[a]
dimethyl ether	2.69	0	0	0	0	0	0	1	0	0	6.79	1.98	-2.55	-2.76	-1.90	[a]
methyl tert-butylether	3.97	2	0	0	0	0	0	1	0	0	7.61	-0.37	-1.54	-1.52	-2.21	[a]
methylethyl ether	3.26	0	0	0	0	0	0	1	0	0	8.03	2.08	-2.18	-2.30	-2.01	[a]
polyfragment solutes																
1,1,1,2-tetrachloroethane	4.29	2	0	0	0	0	4	0	0	0	12.92	6.27	-3.42	-2.86	-1.28	[b]
1,1,1-trichloroethane	3.86	2	0	0	0	0	3	0	0	0	11.71	5.53	-1.89	-1.49	-0.19	[b]
1,1,2,2-tetrachloroethane	4.19	2	0	0	0	0	4	0	0	0	12.11	5.46	-4.07	-3.74	-2.47	[b]
1,1,2-trichloroethane	3.77	1	0	0	0	0	3	0	0	0	8.99	2.90	-5.52	-5.57	-1.99	[b]
1,1-dichloroethane	3.35	1	0	0	0	0	2	0	0	0	10.15	4.93	-1.64	-1.41	-0.85	[b]
1,1-dichloroethene	3.20	1	1	0	0	0	2	0	0	0	11.44	6.92	-1.03	-0.75	0.25	[b]
1,2,3,4-tetrachlorobenzene	5.13	4	0	1	0	0	4	0	0	0	11.88	3.66	-5.29	-4.19	-1.34	[b]
1,2,3,5-tetrachlorobenzene	5.14	4	0	1	0	0	4	0	0	0	12.37	4.07	-4.81	-3.78	-1.62	[b]
1,2,3-trichlorobenzene	4.75	3	0	1	0	0	3	0	0	0	12.09	4.60	-3.48	-2.50	-1.24	[b]
1,2,4,5-tetrachlorobenzene	5.17	4	0	1	0	0	4	0	0	0	12.59	4.26	-4.64	-3.57	-1.34	[b]
1,2,4-trichlorobenzene	4.83	3	0	1	0	0	3	0	0	0	12.90	5.31	-2.78	-1.74	-1.12	[b]
1,2-dichlorobenzene	4.34	2	0	1	0	0	2	0	0	0	11.77	4.95	-2.14	-1.41	-1.41	[b]
1,2-dichloroethane	3.34	0	0	0	0	0	2	0	0	0	10.03	4.66	-2.81	-3.07	-1.77	[b]
1,2-dichloropropane	3.78	1	0	0	0	0	2	0	0	0	9.67	3.25	-2.76	-2.82	-1.27	[b]
1,2-dimethoxyethane	4.01	0	0	0	0	0	0	2	0	0	8.10	0.09	-4.94	-5.19	-4.84	[b]
1,2-ethanediol	2.53	0	0	0	2	0	0	0	0	0	-2.83	-11.81	-8.77	-8.64	-7.75	[b]
1,3,5-trichlorobenzene	4.84	3	0	1	0	0	3	0	0	0	13.37	5.73	-2.33	-1.32	-0.78	[b]
1,3-dichlorobenzene	4.39	2	0	1	0	0	2	0	0	0	12.46	5.58	-1.51	-0.75	-0.98	[b]
1,3-dichloropropane	3.83	0	0	0	0	0	2	0	0	0	9.47	2.83	-4.11	-4.59	-1.90	[b]
1,4-dichlorobenzene	4.40	2	0	1	0	0	2	0	0	0	12.52	5.62	-1.49	-0.70	-1.01	[b]
1,4-dichloropentane	4.76	1	0	0	0	0	2	0	0	0	11.24	2.60	-2.67	-2.84	-2.32	[b]
2,3-dimethylbuta-1,3-diene	4.04	2	2	0	0	0	0	0	0	0	11.35	4.72	1.95	2.52	0.40	[b]
2-butoxyethanol	4.85	0	0	0	1	0	0	1	0	0	5.23	-6.73	-6.64	-6.78	-6.26	[b]
2-chlorophenol	3.95	2	0	1	1	1	1	0	0	0	3.35	-5.35	-8.66	-8.59	-2.82	[b]
2-chlorotoluene	4.51	2	0	1	0	0	1	0	0	0	11.94	4.54	-0.12	0.68	-1.14	[b]
2-ethoxyethanol	3.82	0	0	0	1	0	0	1	0	0	3.22	-6.47	-7.09	-7.17	-6.70	[b]
2-methoxyphenol	4.29	2	0	1	1	1	0	1	0	0	2.25	-7.71	-9.85	-9.72	-5.58	[b]
2-methylbuta-1,3-diene	3.65	1	2	0	0	0	0	0	0	0	11.01	5.25	1.13	1.42	0.68	[b]
2-methylstyrene	4.87	2	1	1	0	0	0	0	0	0	10.66	2.06	-0.77	-0.42	-1.24	[b]

2-phenylethanol	4.61	1	0	1	1	0	0	0	0	0	3.81	-7.25	-6.63	-6.72	-6.80	[b]
2-propoxyethanol	4.33	0	0	0	1	0	0	1	0	0	4.40	-6.37	-6.70	-6.75	-6.41	[b]
3-chlorophenol	4.00	2	0	1	1	1	1	0	0	0	4.95	-3.75	-7.13	-6.95	-6.61	[b]
3-hydroxybenzaldehyde	4.08	2	0	1	1	1	0	0	1	0	1.38	-8.71	-9.62	-9.55	-9.51	[b]
3-methoxyphenol	4.32	2	0	1	1	1	0	1	0	0	3.93	-6.01	-8.22	-7.99	-7.66	[b]
3-phenylpropanol	5.12	1	0	1	1	0	0	0	0	0	2.96	-9.42	-8.25	-8.57	-6.93	[b]
4-chloro-3-methylphenol	4.48	3	0	1	1	1	1	0	0	0	5.42	-4.38	-6.31	-5.89	-6.79	[b]
4-chlorophenol	4.03	2	0	1	1	1	1	0	0	0	5.08	-3.66	-7.04	-6.85	-7.04	[b]
4-hydroxybenzaldehyde	4.08	2	0	1	1	1	0	0	1	0	0.98	-9.15	-10.03	-9.98	-9.65	[b]
4-methoxyacetophenone	5.19	3	0	1	0	0	0	1	0	1	8.09	-2.29	-5.96	-5.34	-4.40	[b]
E-but-2-enal	3.37	0	1	0	0	0	0	0	1	0	7.04	0.77	-3.47	-3.47	-4.23	[b]
E-hex-2-enal	4.43	0	1	0	0	0	0	0	1	0	9.09	0.50	-3.01	-3.07	-3.68	[b]
E-oct-2-enal	5.43	0	1	0	0	0	0	0	1	0	10.58	-0.25	-3.04	-3.18	-3.44	[b]
acetophenone	4.47	2	0	1	0	0	0	0	0	1	7.59	-1.16	-4.75	-4.68	-4.54	[b]
allyl alcohol	2.88	0	1	0	1	0	0	0	0	0	1.81	-5.35	-6.31	-6.50	-5.10	[b]
benzyl alcohol	4.12	1	0	1	1	0	0	0	0	0	2.52	-7.21	-7.19	-6.99	-6.63	[b]
buta-1,3-diene	3.20	0	2	0	0	0	0	0	0	0	10.47	5.62	0.20	0.12	0.61	[b]
chlorobenzene	4.01	1	0	1	0	0	1	0	0	0	11.44	5.11	-0.93	-0.46	-1.09	[b]
cis-1,2-dichloroethene	3.12	0	1	0	0	0	2	0	0	0	9.47	4.83	-3.96	-4.28	-0.93	[b]
dichloromethane	2.84	0	0	0	0	0	2	0	0	0	8.93	4.63	-3.15	-3.43	-1.31	[b]
dimethoxymethane	3.52	0	0	0	0	0	0	2	0	0	6.66	-0.30	-5.63	-5.90	-2.97	[b]
ethyl phenyl ether	4.93	1	0	1	0	0	0	1	0	0	11.49	2.79	-1.87	-1.18	-2.22	[b]
hexa-1,5-diene	4.27	0	2	0	0	0	0	0	0	0	12.45	5.28	0.57	0.46	1.01	[b]
methyl_phenyl_ether	4.37	1	0	1	0	0	0	1	0	0	10.33	2.74	-2.19	-1.59	-2.45	[b]
penta-1,4-diene	3.76	0	2	0	0	0	0	0	0	0	11.74	5.73	0.62	0.58	0.93	[b]
pentachloroethane	4.70	3	0	0	0	0	5	0	0	0	14.01	6.77	-3.98	-3.11	-1.39	[b]
tetrachloroethene	4.08	2	1	0	0	0	4	0	0	0	13.88	8.09	-3.06	-2.41	0.10	[b]
tetrachloromethane	3.84	2	0	0	0	0	4	0	0	0	13.21	7.55	-2.45	-1.87	0.08	[b]
trans-1,2-dichloroethene	3.17	0	1	0	0	0	2	0	0	0	10.85	6.18	-2.65	-2.90	-0.78	[b]
trichloroethene	3.63	1	1	0	0	0	3	0	0	0	12.13	6.87	-3.10	-2.91	-0.44	[b]
trichloromethane	3.36	1	0	0	0	0	3	0	0	0	10.95	5.84	-2.94	-2.88	-1.08	[b]

[a] – training set; [b] – test set;

For ref. [1], [7] value of $\Delta\mu_{hyd}^{\exp}$ was recalculated from logP (water/gas) as: $\Delta\mu_{hyd}^{\exp} = -10^{-3} \ln 10 \cdot RT \log P(water/gas)$ (S-1)