Small molecule hydration free energies in explicit solvent: An extensive test of atomistic simulations: Supporting Information

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Table 1 shows the full computed ($\Delta G_{hyd.}$) and experimental ($\Delta G_{expt.}$) hydration free energies for all of the compounds in the test set with the original GAFF parameters. It includes the breakdown into electrostatic components ($\Delta G_{elec.}$) and nonpolar components ($\Delta G_{vdw.}$). Computed uncertainties are provided.

TABLE 1:: Computed and experimental hydration free energies and components.

Molecule name	$\Delta G_{elec.}$	$\Delta G_{vdw.}$	$\Delta G_{hyd.}$	$\Delta G_{expt.}$
1112_tetrachloroethane	-1.43 ± 0.01	1.54 ± 0.02	0.11 ± 0.02	-1.28
111_trichloroethane	-1.13 ± 0.00	1.88 ± 0.02	0.75 ± 0.02	-0.19
111_trifluoro_222_trimethoxyethane	-4.57 ± 0.01	2.31 ± 0.02	-2.26 ± 0.02	-0.80
111_trifluoropropan_2_ol	-6.05 ± 0.02	2.49 ± 0.02	-3.56 ± 0.03	-4.16
111_trimethoxyethane	-5.55 ± 0.01	1.66 ± 0.02	-3.89 ± 0.02	-4.42
1122_tetrachloroethane	-1.88 ± 0.03	1.47 ± 0.02	-0.41 ± 0.04	-2.47
112_trichloro_122_trifluoroethane	-0.32 ± 0.00	1.85 ± 0.02	1.53 ± 0.02	1.77
112_trichloroethane	-2.01 ± 0.02	1.51 ± 0.02	-0.50 ± 0.03	-1.99
11_diacetoxyethane	-9.52 ± 0.09	1.62 ± 0.03	-7.90 ± 0.10	-4.97
11_dichloroethane	-1.64 ± 0.01	1.81 ± 0.02	0.17 ± 0.02	-0.84
11_dichloroethene	-0.85 ± 0.00	2.09 ± 0.02	1.24 ± 0.02	0.25
11_diethoxyethane	-4.57 ± 0.01	2.39 ± 0.02	-2.18 ± 0.02	-3.28
11_difluoroethane	-2.41 ± 0.01	2.60 ± 0.02	0.19 ± 0.02	-0.11
1234_tetrachlorobenzene	-1.25 ± 0.01	0.93 ± 0.02	-0.32 ± 0.02	-1.34
1235_tetrachlorobenzene	-0.92 ± 0.00	0.90 ± 0.02	-0.02 ± 0.02	-1.62
123_trichlorobenzene	-1.67 ± 0.01	1.29 ± 0.02	-0.38 ± 0.02	-1.24
123_trimethylbenzene	-2.79 ± 0.01	2.14 ± 0.02	-0.65 ± 0.02	-1.21
1245_tetrachlorobenzene	-0.97 ± 0.00	1.22 ± 0.02	0.25 ± 0.02	-1.34
124_trichlorobenzene	-1.35 ± 0.00	1.17 ± 0.02	-0.18 ± 0.02	-1.12
124_trimethylbenzene	-2.75 ± 0.01	2.39 ± 0.02	-0.36 ± 0.02	-0.86
12_diacetoxyethane	-9.93 ± 0.02	1.61 ± 0.03	-8.32 ± 0.04	-6.34
12_dibromoethane	-1.60 ± 0.01	1.79 ± 0.02	0.19 ± 0.02	-2.33
12_dichlorobenzene	-1.96 ± 0.01	1.32 ± 0.02	-0.64 ± 0.02	-1.36
12_dichloroethane	-2.15 ± 0.01	1.63 ± 0.02	-0.52 ± 0.02	-1.79
12_dichloropropane	-2.13 ± 0.01	1.93 ± 0.02	-0.20 ± 0.02	-1.27
12_diethoxyethane	-5.47 ± 0.01	2.39 ± 0.03	-3.08 ± 0.03	-3.54
12_dimethoxyethane	-5.29 ± 0.01	1.93 ± 0.02	-3.36 ± 0.02	-4.84
12_ethanediol	-8.71 ± 0.02	1.09 ± 0.02	-7.62 ± 0.03	-9.30
135_trichlorobenzene	-0.96 ± 0.00	1.41 ± 0.02	0.45 ± 0.02	-0.78
135_trimethylbenzene	-2.73 ± 0.01	2.77 ± 0.02	0.04 ± 0.02	-0.90
13_dichlorobenzene	-1.60 ± 0.01	1.61 ± 0.02	0.01 ± 0.02	-0.98
13_dichloropropane	-2.18 ± 0.01	1.80 ± 0.02	-0.38 ± 0.02	-1.89
13_dimethylnaphthalene	-4.50 ± 0.01	1.71 ± 0.03	-2.79 ± 0.03	-2.47
14_dichlorobenzene	-1.63 ± 0.01	1.53 ± 0.02	-0.10 ± 0.02	-1.01
14_dichlorobutane	-2.38 ± 0.01	2.11 ± 0.02	-0.27 ± 0.02	-2.32
14_dimethyl_piperazine	-8.20 ± 0.02	0.80 ± 0.02	-7.40 ± 0.03	-7.58
14_dimethylnaphthalene	-4.50 ± 0.01	1.21 ± 0.03	-3.29 ± 0.03	-2.82
14_dioxane	-4.71 ± 0.01	0.36 ± 0.02	-4.35 ± 0.02	-5.06
1_bromo_2_chloroethane	-1.77 ± 0.01	1.79 ± 0.02	0.02 ± 0.02	-1.95
1_bromo_2_methylpropane	-0.95 ± 0.01	2.19 ± 0.02	1.24 ± 0.02	-0.03
1_bromobutane	-0.97 ± 0.00	2.65 ± 0.02	1.68 ± 0.02	-0.40
1_bromoheptane	-0.97 ± 0.00	2.63 ± 0.03	1.66 ± 0.03	0.34
1_bromohexane	-0.97 ± 0.00	2.75 ± 0.02	1.78 ± 0.02	0.18

1_bromooctane	-0.97 ± 0.00	2.89 ± 0.03	1.92 ± 0.03	0.52
1_bromopentane	-0.96 ± 0.00	2.44 ± 0.02	1.48 ± 0.02	-0.10
1_bromopropane	-0.98 ± 0.00	2.27 ± 0.02	1.29 ± 0.02	-0.56
1_chloro_222_trifluoroethane	-2.27 ± 0.01	2.43 ± 0.02	0.16 ± 0.02	0.06
1_chlorobutane	-1.22 ± 0.01	2.21 ± 0.02	0.99 ± 0.02	-0.16
1_chloroheptane	-1.21 ± 0.00	2.74 ± 0.03	1.53 ± 0.03	0.29
1_chlorohexane	-1.23 ± 0.01	2.46 ± 0.03	1.23 ± 0.03	0.00
1_chloropentane	-1.22 ± 0.01	2.40 ± 0.02	1.18 ± 0.02	-0.07
1_chloropropane	-1.25 ± 0.00	2.17 ± 0.02	0.92 ± 0.02	-0.33
1_ethylnaphthalene	-4.61 ± 0.01	1.61 ± 0.03	-3.00 ± 0.03	-2.40
1_iodobutane	-1.83 ± 0.01	2.41 ± 0.02	0.58 ± 0.02	-0.25
1_iodoheptane	-1.80 ± 0.01	2.99 ± 0.03	1.19 ± 0.03	0.27
1_iodohexane	-1.81 ± 0.01	2.47 ± 0.02	0.66 ± 0.02	0.08
1_iodopentane	-1.82 ± 0.01	2.48 ± 0.02	0.66 ± 0.02	-0.14
1_iodopropane	-1.87 ± 0.01	1.87 ± 0.02	0.00 ± 0.02	-0.53
1_methyl_imidazole	-7.06 ± 0.02	0.73 ± 0.02	-6.33 ± 0.03	-8.41
1_methyl_pyrrole	-3.90 ± 0.01	1.31 ± 0.02	-2.59 ± 0.02	-2.89
1_methylcyclohexene	-0.66 ± 0.00	1.99 ± 0.02	1.33 ± 0.02	0.67
1_methylnaphthalene	-4.52 ± 0.01	1.28 ± 0.02	-3.24 ± 0.02	-2.44
1_naphthol	-8.31 ± 0.02	0.80 ± 0.02	-7.51 ± 0.03	-7.67
1_naphthylamine	-8.63 ± 0.02	0.87 ± 0.02	-7.76 ± 0.03	-7.28
1_nitrobutane	-2.43 ± 0.01	0.92 ± 0.02	-1.51 ± 0.02	-3.09
1_nitropentane	-2.40 ± 0.01	1.11 ± 0.02	-1.29 ± 0.02	-2.82
1_nitropropane	-2.44 ± 0.01	1.06 ± 0.02	-1.38 ± 0.02	-3.34
222_trifluoroethanol	-6.05 ± 0.02	2.10 ± 0.02	-3.95 ± 0.03	-4.31
224_trimethylpentane	0.02 ± 0.00	2.91 ± 0.03	2.93 ± 0.03	2.89
225_trimethylhexane	0.00 ± 0.00	2.86 ± 0.03	2.86 ± 0.03	2.93
22_dimethylbutane	0.01 ± 0.00	2.52 ± 0.02	2.53 ± 0.02	2.51
22_dimethylpentane	0.01 ± 0.00	2.89 ± 0.02	2.90 ± 0.02	2.88
22_dimethylpropane	0.01 ± 0.00	2.59 ± 0.02	2.60 ± 0.02	2.51
234_trimethylpentane	0.01 ± 0.00	2.85 ± 0.03	2.86 ± 0.03	2.56
23_dimethylbuta_13_diene	-1.11 ± 0.01	2.80 ± 0.02	1.69 ± 0.02	0.40
23_dimethylbutane	0.01 ± 0.00	2.68 ± 0.02	2.69 ± 0.02	2.34
23_dimethylnaphthalene	-4.43 ± 0.01	1.84 ± 0.02	-2.59 ± 0.02	-2.78
23_dimethylpentane	0.00 ± 0.00	2.66 ± 0.03	2.66 ± 0.03	2.52
23_dimethylphenol	-6.49 ± 0.02	1.82 ± 0.02	-4.67 ± 0.03	-6.16
23_dimethylpyridine	-4.79 ± 0.01	1.52 ± 0.02	-3.27 ± 0.02	-4.82
24_dimethylpentan_3_one	-5.13 ± 0.01	2.66 ± 0.02	-2.47 ± 0.02	-2.74
24_dimethylpentane	0.00 ± 0.00	2.89 ± 0.03	2.89 ± 0.03	2.83
24_dimethylphenol	-6.48 ± 0.02	1.93 ± 0.02	-4.55 ± 0.03	-6.01
24_dimethylpyridine	-4.94 ± 0.01	1.76 ± 0.02	-3.18 ± 0.02	-4.86
25_dimethylphenol	-5.97 ± 0.02	1.58 ± 0.02	-4.39 ± 0.03	-5.91
25_dimethylpyridine	-4.76 ± 0.01	1.93 ± 0.02	-2.83 ± 0.02	-4.72
25_dimethyltetrahydrofuran	-3.52 ± 0.01	1.63 ± 0.02	-1.89 ± 0.02	-2.92
26_dimethylaniline	-6.51 ± 0.02	1.64 ± 0.02	-4.87 ± 0.03	-5.21
26_dimethylnaphthalene	-4.42 ± 0.01	1.77 ± 0.03	-2.65 ± 0.03	-2.63
26_dimethylphenol	-5.78 ± 0.02	1.69 ± 0.02	-4.09 ± 0.03	-5.26
26_dimethylpyridine	-5.15 ± 0.01	1.79 ± 0.02	-3.36 ± 0.02	-4.59
2_bromo_2_methylpropane	-1.25 ± 0.01	2.14 ± 0.02	0.89 ± 0.02	0.84
2_bromopropane	-1.16 ± 0.01	2.13 ± 0.02	0.97 ± 0.02	-0.48
2_butoxyethanol	-5.94 ± 0.02	1.87 ± 0.02	-4.07 ± 0.03	-6.25
2_chloro_111_trimethoxyethane	-5.40 ± 0.02	2.10 ± 0.03	-3.30 ± 0.04	-4.59
2_chloro_2_methylpropane	-1.44 ± 0.01	2.26 ± 0.02	0.82 ± 0.02	1.09
2_chloroaniline	-6.04 ± 0.02	1.08 ± 0.02	-4.96 ± 0.03	-4.91
2_chlorobutane	-1.35 ± 0.00	2.56 ± 0.02	1.21 ± 0.02	0.00
2_chlorophenol	-4.51 ± 0.02	1.28 ± 0.02	-3.23 ± 0.03	-4.55
2_chloropropane	-1.40 ± 0.01	2.22 ± 0.02	0.82 ± 0.02	-0.25
2_chloropyridine	-4.85 ± 0.01	1.49 ± 0.02	-3.36 ± 0.02	-4.39
2_chlorotoluene	-2.18 ± 0.01	1.67 ± 0.02	-0.51 ± 0.02	-1.14
2_ethoxyethanol	-6.41 ± 0.02	1.64 ± 0.02	-4.77 ± 0.03	-6.69
2_ethylpyrazine	-6.94 ± 0.02	1.26 ± 0.02	-5.68 ± 0.03	-5.45

2_ethylpyridine	-4.96 ± 0.01	1.75 ± 0.02	-3.21 ± 0.02	-4.33
2_ethyltoluene	-2.85 ± 0.01	2.19 ± 0.03	-0.66 ± 0.03	-1.04
2_fluorophenol	-4.89 ± 0.03	1.65 ± 0.02	-3.24 ± 0.03	-5.29
2_iodophenol	-3.93 ± 0.03	1.02 ± 0.02	-2.91 ± 0.03	-6.20
2_iodopropane	-1.97 ± 0.01	2.26 ± 0.02	0.29 ± 0.02	-0.46
2_isobutylpyrazine	-6.81 ± 0.01	1.71 ± 0.03	-5.10 ± 0.03	-5.04
2_methoxy_111_trimethoxyethane	-7.61 ± 0.02	1.64 ± 0.03	-5.97 ± 0.04	-5.73
2_methoxyaniline	-7.69 ± 0.02	1.16 ± 0.02	-6.53 ± 0.03	-6.12
2_methoxyethanamine	-7.04 ± 0.02	1.42 ± 0.02	-5.62 ± 0.03	-6.55
2_methoxyethanol	-6.92 ± 0.02	1.55 ± 0.02	-5.37 ± 0.03	-6.76
2_methoxyphenol	-6.00 ± 0.02	1.26 ± 0.02	-4.74 ± 0.03	-5.57
2_methyl_but_2_ene	-0.56 ± 0.00	2.94 ± 0.02	2.38 ± 0.02	1.31
2_methylbut_2_ene	-0.55 ± 0.00	2.83 ± 0.02	2.28 ± 0.02	1.31
2_methylbuta_13_diene	-1.12 ± 0.01	2.93 ± 0.02	1.81 ± 0.02	0.68
2_methylbutan_1_ol	-4.88 ± 0.01	2.10 ± 0.02	-2.78 ± 0.02	-4.42
2_methylbutan_2_ol	-5.17 ± 0.02	2.21 ± 0.02	-2.96 ± 0.03	-4.43
2_methylbutane	0.01 ± 0.00	2.51 ± 0.02	2.52 ± 0.02	2.38
2_methylhexane	0.01 ± 0.00	2.99 ± 0.03	3.00 ± 0.03	2.93
2_methylpent_1_ene	-0.40 ± 0.00	3.15 ± 0.02	2.75 ± 0.02	1.47
2_methylpentan_2_ol	-5.13 ± 0.01	2.34 ± 0.02	-2.79 ± 0.02	-3.92
2_methylpentan_3_ol	-4.75 ± 0.02	2.56 ± 0.02	-2.19 ± 0.03	-3.88
2_methylpentane	0.01 ± 0.00	2.77 ± 0.02	2.78 ± 0.02	2.51
2_methylpropan_1_ol	-5.02 ± 0.01	2.06 ± 0.02	-2.96 ± 0.02	-4.50
2_methylpropan_2_ol	-5.31 ± 0.01	2.22 ± 0.02	-3.09 ± 0.02	-4.47
2_methylpropane	0.01 ± 0.00	2.73 ± 0.02	2.74 ± 0.02	2.32
2_methylpropene	-0.45 ± 0.00	2.79 ± 0.02	2.34 ± 0.02	1.16
2_methylpyrazine	-6.99 ± 0.02	0.89 ± 0.02	-6.10 ± 0.03	-5.51
2_methylpyridine	-4.95 ± 0.01	1.54 ± 0.02	-3.41 ± 0.02	-4.63
2_methyltetrahydrofuran	-3.39 ± 0.01	1.44 ± 0.02	-1.95 ± 0.02	-3.30
2_methylthiophene	-1.90 ± 0.01	1.68 ± 0.02	-0.22 ± 0.02	-1.38
2_naphthol	-8.70 ± 0.02	0.82 ± 0.02	-7.88 ± 0.03	-8.11
2_naphthylamine	-8.83 ± 0.02	0.96 ± 0.02	-7.87 ± 0.03	-7.47
2_nitroaniline	-7.84 ± 0.02	-0.12 ± 0.02	-7.96 ± 0.03	-7.37
2_nitrophenol	-5.40 ± 0.02	0.06 ± 0.02	-5.34 ± 0.03	-4.58
2_nitropropane	-2.54 ± 0.01	0.93 ± 0.02	-1.61 ± 0.02	-3.13
2_nitrotoluene	-3.79 ± 0.01	0.65 ± 0.02	-3.14 ± 0.02	-3.58
2_phenylethanol	-7.05 ± 0.02	1.72 ± 0.02	-5.33 ± 0.03	-6.79
2_propoxyethanol	-6.14 ± 0.02	1.93 ± 0.02	-4.21 ± 0.03	-6.40
333_trimethoxypropionitrile	-6.88 ± 0.02	1.95 ± 0.03	-4.93 ± 0.04	-6.40
33_dimethylbutan_2_one	-5.18 ± 0.01	2.27 ± 0.02	-2.91 ± 0.02	-3.11
33_dimethylpentane	0.01 ± 0.00	2.52 ± 0.03	2.53 ± 0.03	2.56
34_dimethylphenol	-6.86 ± 0.02	1.53 ± 0.02	-5.33 ± 0.03	-6.50
34_dimethylpyridine	-4.59 ± 0.01	1.41 ± 0.02	-3.18 ± 0.02	-5.22
35_dimethylphenol	-7.01 ± 0.02	1.89 ± 0.02	-5.12 ± 0.03	-6.27
35_dimethylpyridine	-4.47 ± 0.01	1.53 ± 0.02	-2.94 ± 0.02	-4.84
3_acetylpyridine	-8.04 ± 0.02	0.94 ± 0.02	-7.10 ± 0.03	-8.26
3_chloroaniline	-6.41 ± 0.01	1.04 ± 0.02	-5.37 ± 0.02	-5.82
3_chlorophenol	-6.38 ± 0.02	1.10 ± 0.02	-5.28 ± 0.03	-6.62
3_chloroprop_1_ene	-1.48 ± 0.01	2.36 ± 0.02	0.88 ± 0.02	-0.57
3_chloropyridine	-3.78 ± 0.01	1.28 ± 0.02	-2.50 ± 0.02	-4.01
3_cyanophenol	-8.16 ± 0.02	1.12 ± 0.02	-7.04 ± 0.03	-9.65
3_cyanopyridine	-5.79 ± 0.01	1.13 ± 0.02	-4.66 ± 0.02	-6.75
3_ethylphenol	-6.91 ± 0.02	1.89 ± 0.02	-5.02 ± 0.03	-6.25
3_ethylpyridine	-4.59 ± 0.01	1.63 ± 0.02	-2.96 ± 0.02	-4.59
3_formylpyridine	-8.22 ± 0.02	0.58 ± 0.02	-7.64 ± 0.03	-7.10
3_hydroxybenzaldehyde	-10.18 ± 0.02	0.94 ± 0.02	-9.24 ± 0.03	-9.50
3_methoxyaniline	-8.44 ± 0.02	0.99 ± 0.02	-7.45 ± 0.03	-7.29
3_methoxyphenol	-8.10 ± 0.02	1.07 ± 0.02	-7.03 ± 0.03	-7.66
3_methyl_1h_indole	-7.53 ± 0.02	0.98 ± 0.02	-6.55 ± 0.03	-5.88
3_methyl_but_1_ene	-0.33 ± 0.00	3.13 ± 0.02	2.80 ± 0.02	1.83
3_methylbut_1_ene	-0.34 ± 0.00	3.01 ± 0.02	2.67 ± 0.02	1.82

3_methylbutan_1_ol	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-4.42
3_methylbutan_2_one	-5.34 ± 0.01	2.41 ± 0.02	-2.93 ± 0.02	-3.24
3_methylbutanoic_acid	-6.99 ± 0.02	1.48 ± 0.02	-5.51 ± 0.03	-6.09
3_methylheptane	0.01 ± 0.00	3.28 ± 0.03	3.29 ± 0.03	2.97
3_methylhexane	0.00 ± 0.00	2.76 ± 0.02	2.76 ± 0.02	2.71
3_methylpentane	0.00 ± 0.00	2.72 ± 0.02	2.72 ± 0.02	2.51
3_methylpyridine	-4.56 ± 0.01	1.37 ± 0.02	-3.19 ± 0.02	-4.77
3_nitroaniline	-8.00 ± 0.02	-0.24 ± 0.02	-8.24 ± 0.03	-8.84
3_nitrophenol	-7.45 ± 0.02	-0.21 ± 0.02	-7.66 ± 0.03	-9.62
3_nitrotoluene	-3.51 ± 0.01	0.35 ± 0.02	-3.16 ± 0.02	-3.45
3_phenylpropanol	-7.38 ± 0.03	1.88 ± 0.02	-5.50 ± 0.03	-6.92
4_acetylpyridine	-8.38 ± 0.02	0.75 ± 0.02	-7.63 ± 0.03	-7.62
4_bromophenol	-6.59 ± 0.01	1.12 ± 0.02	-5.47 ± 0.02	-7.13
4_bromotoluene	-2.20 ± 0.01	2.24 ± 0.02	0.04 ± 0.02	-1.39
4_chloro_3_methylphenol	-6.38 ± 0.02	1.48 ± 0.02	-4.90 ± 0.03	-6.79
4_chloroaniline	-6.47 ± 0.01	1.19 ± 0.02	-5.28 ± 0.02	-5.90
4_chlorophenol	-6.53 ± 0.01	1.17 ± 0.02	-5.36 ± 0.02	-7.03
4_cyanophenol	-8.72 ± 0.02	1.11 ± 0.02	-7.61 ± 0.03	-10.17
4_cyanopyridine	-5.99 ± 0.01	1.02 ± 0.02	-4.97 ± 0.02	-6.02
4_ethylphenol	-7.07 ± 0.02	1.99 ± 0.02	-5.08 ± 0.03	-6.13
4_ethylpyridine	-4.72 ± 0.01	1.85 ± 0.02	-2.87 ± 0.02	-4.73
4_ethyltoluene	-2.78 ± 0.01	2.73 ± 0.02	-0.05 ± 0.02	-0.95
4_fluorophenol	-6.51 ± 0.02	1.52 ± 0.02	-4.99 ± 0.03	-6.19
4_formylpyridine	-8.13 ± 0.02	0.82 ± 0.02	-7.31 ± 0.03	-7.00
4_hydroxybenzaldehyde	-10.85 ± 0.02	0.85 ± 0.02	-10.00 ± 0.03	-8.83
4_isopropyltoluene	-2.53 ± 0.01	2.73 ± 0.03	0.20 ± 0.03	-0.68
4_methoxyacetophenone	-7.89 ± 0.01	1.60 ± 0.03	-6.29 ± 0.03	-4.40
4_methoxyaniline	-8.09 ± 0.02	1.17 ± 0.02	-6.92 ± 0.03	-7.48
4_methyl_1h_imidazole	-8.85 ± 0.02	0.86 ± 0.02	-7.99 ± 0.03	-10.27
4_methylacetophenone	-6.70 ± 0.02	1.88 ± 0.02	-4.82 ± 0.03	-4.70
4_methylbenzaldehyde	-6.43 ± 0.02	1.53 ± 0.02	-4.90 ± 0.03	-4.27
4_methylpentan_2_ol	-5.10 ± 0.01	2.35 ± 0.02	-2.75 ± 0.02	-3.73
4_methylpentan_2_one	-5.28 ± 0.01	2.32 ± 0.02	-2.96 ± 0.02	-3.05
4_methylpyridine	-4.73 ± 0.01	1.32 ± 0.02	-3.41 ± 0.02	-4.93
4_n_propylphenol	-6.96 ± 0.01	1.46 ± 0.02	-5.50 ± 0.02	-5.90
4_nitroaniline	-9.03 ± 0.02	-0.20 ± 0.02	-9.23 ± 0.03	-10.27
4_nitrophenol	-8.04 ± 0.01	-0.18 ± 0.02	-8.22 ± 0.02	-10.64
4_tert_butylphenol	-7.21 ± 0.02	1.67 ± 0.03	-5.54 ± 0.04	-5.91
E_12_dichloroethene	-0.87 ± 0.00	2.07 ± 0.02	1.20 ± 0.02	-0.78
E_but_2_enal	-5.82 ± 0.01	2.16 ± 0.02	-3.66 ± 0.02	-4.22
E_hept_2_ene	-0.43 ± 0.00	3.26 ± 0.02	2.83 ± 0.02	1.68
E_hex_2_enal	-5.48 ± 0.01	2.26 ± 0.02	-3.22 ± 0.02	-3.68
E_oct_2_enal	-5.37 ± 0.01	2.90 ± 0.03	-2.47 ± 0.03	-3.43
NN_dimethyl_p_methoxybenzamide	-10.16 ± 0.02	0.87 ± 0.04	-9.29 ± 0.04	-11.01
NN_dimethyl_p_methylbenzamide	-9.10 ± 0.02	1.59 ± 0.04	-7.51 ± 0.04	-9.76
NN_dimethyl_p_nitrobenzamide	-9.24 ± 0.02	-0.68 ± 0.03	-9.92 ± 0.04	-11.95
NN_dimethylaniline	-6.13 ± 0.01	1.43 ± 0.02	-4.70 ± 0.02	-3.45
NN_dimethylbenzamide	-9.17 ± 0.02	1.19 ± 0.03	-7.98 ± 0.04	-9.29
NN_dimethylformamide	-8.13 ± 0.02	1.27 ± 0.02	-6.86 ± 0.03	-7.81
N_acetylpyrrolidine	-8.86 ± 0.01	0.89 ± 0.02	-7.97 ± 0.02	-9.80
N_methyl_N__222_trifluoroethyl__aniline	-6.24 ± 0.01	2.55 ± 0.03	-3.69 ± 0.03	-1.92
N_methylacetamide	-9.93 ± 0.02	1.54 ± 0.02	-8.39 ± 0.03	-10.00
N_methylaniline	-7.10 ± 0.02	1.36 ± 0.02	-5.74 ± 0.03	-4.69
N_methylmorpholine	-6.46 ± 0.02	0.59 ± 0.02	-5.87 ± 0.03	-6.32
N_methylpiperazine	-8.40 ± 0.02	0.10 ± 0.02	-8.30 ± 0.03	-7.77
N_methylpiperidine	-4.18 ± 0.01	0.97 ± 0.02	-3.21 ± 0.02	-3.88
Z_12_dichloroethene	-1.72 ± 0.01	2.03 ± 0.02	0.31 ± 0.02	-1.17
Z_pent_2_ene	-0.42 ± 0.00	2.97 ± 0.02	2.55 ± 0.02	1.31
acenaphthene	-4.89 ± 0.01	1.38 ± 0.03	-3.51 ± 0.03	-3.15
acetaldehyde	-5.18 ± 0.01	1.79 ± 0.02	-3.39 ± 0.02	-3.50
acetic_acid	-7.07 ± 0.02	1.12 ± 0.01	-5.95 ± 0.02	-6.69

acetonitrile	-3.77 ± 0.01	2.10 ± 0.01	-1.67 ± 0.01	-3.88
acetophenone	-6.67 ± 0.02	1.60 ± 0.02	-5.07 ± 0.03	-4.58
alpha_methylstyrene	-3.53 ± 0.01	2.27 ± 0.02	-1.26 ± 0.02	-1.24
ammonia	-5.82 ± 0.01	1.78 ± 0.01	-4.04 ± 0.01	-4.29
aniline	-7.00 ± 0.01	1.08 ± 0.02	-5.92 ± 0.02	-5.49
anisole	-3.98 ± 0.01	1.68 ± 0.02	-2.30 ± 0.02	-2.45
anthracene	-5.97 ± 0.01	0.58 ± 0.03	-5.39 ± 0.03	-3.95
azetidine	-5.09 ± 0.01	1.68 ± 0.02	-3.41 ± 0.02	-5.56
benzaldehyde	-6.36 ± 0.01	1.37 ± 0.02	-4.99 ± 0.02	-4.02
benzamide	-10.97 ± 0.02	0.78 ± 0.02	-10.19 ± 0.03	-11.00
benzene	-2.70 ± 0.01	2.00 ± 0.02	-0.70 ± 0.02	-0.86
benzonitrile	-4.13 ± 0.01	1.39 ± 0.02	-2.74 ± 0.02	-4.21
benzotrifluoride	-3.02 ± 0.01	2.47 ± 0.02	-0.55 ± 0.02	-0.25
benzyl_alcohol	-6.94 ± 0.02	1.53 ± 0.02	-5.41 ± 0.03	-6.62
benzyl_bromide	-3.13 ± 0.01	1.99 ± 0.02	-1.14 ± 0.02	-2.38
benzyl_chloride	-3.37 ± 0.01	1.81 ± 0.02	-1.56 ± 0.02	-1.93
biphenyl	-4.97 ± 0.01	1.58 ± 0.02	-3.39 ± 0.02	-2.66
bis_2_chloroethyl__ether	-3.78 ± 0.01	1.92 ± 0.02	-1.86 ± 0.02	-4.23
bromobenzene	-2.20 ± 0.01	1.83 ± 0.02	-0.37 ± 0.02	-1.46
bromoethane	-1.01 ± 0.01	1.94 ± 0.02	0.93 ± 0.02	-0.74
bromomethane	-0.89 ± 0.00	1.98 ± 0.01	1.09 ± 0.01	-0.82
bromotrifluoromethane	-0.38 ± 0.00	2.41 ± 0.02	2.03 ± 0.02	1.79
but_1_ene	-0.37 ± 0.00	2.85 ± 0.02	2.48 ± 0.02	1.38
but_1_yne	-0.86 ± 0.00	2.79 ± 0.02	1.93 ± 0.02	-0.16
buta_13_diene	-0.96 ± 0.01	2.89 ± 0.02	1.93 ± 0.02	0.61
butan_1_ol	-5.12 ± 0.01	1.98 ± 0.02	-3.14 ± 0.02	-4.72
butan_2_ol	-5.20 ± 0.02	2.08 ± 0.02	-3.12 ± 0.03	-4.62
butanenitrile	-3.57 ± 0.01	2.16 ± 0.02	-1.41 ± 0.02	-3.64
butanoic_acid	-6.92 ± 0.02	1.46 ± 0.02	-5.46 ± 0.03	-6.35
butanone	-5.05 ± 0.01	2.08 ± 0.02	-2.97 ± 0.02	-3.71
butyraldehyde	-5.07 ± 0.01	2.06 ± 0.02	-3.01 ± 0.02	-3.18
chlorobenzene	-2.13 ± 0.01	1.53 ± 0.02	-0.60 ± 0.02	-1.12
chlorodifluoromethane	-2.32 ± 0.01	2.28 ± 0.02	-0.04 ± 0.02	-0.50
chloroethane	-1.26 ± 0.01	2.04 ± 0.02	0.78 ± 0.02	-0.63
chloroethylene	-1.06 ± 0.00	2.28 ± 0.02	1.22 ± 0.02	-0.59
chlorofluoromethane	-2.25 ± 0.01	2.03 ± 0.01	-0.22 ± 0.01	-0.77
chloromethane	-1.14 ± 0.01	1.95 ± 0.01	0.81 ± 0.01	-0.55
cis_12_dimethylcyclohexane	0.02 ± 0.00	2.03 ± 0.02	2.05 ± 0.02	1.58
cyanobenzene	-4.14 ± 0.01	1.76 ± 0.02	-2.38 ± 0.02	-4.10
cyclohepta_135_triene	-1.97 ± 0.01	2.12 ± 0.02	0.15 ± 0.02	-0.99
cycloheptanol	-5.14 ± 0.01	0.99 ± 0.05	-4.15 ± 0.05	-5.48
cyclohexane	0.01 ± 0.00	1.66 ± 0.02	1.67 ± 0.02	1.23
cyclohexanol	-5.28 ± 0.01	1.02 ± 0.02	-4.26 ± 0.02	-5.46
cyclohexanone	-5.14 ± 0.01	1.30 ± 0.02	-3.84 ± 0.02	-4.91
cyclohexene	-0.53 ± 0.00	2.09 ± 0.02	1.56 ± 0.02	0.37
cyclohexylamine	-5.08 ± 0.01	1.14 ± 0.02	-3.94 ± 0.02	-4.59
cyclopentane	0.01 ± 0.00	1.52 ± 0.02	1.53 ± 0.02	1.20
cyclopentanol	-5.27 ± 0.01	1.12 ± 0.02	-4.15 ± 0.02	-5.49
cyclopentanone	-4.85 ± 0.01	1.14 ± 0.02	-3.71 ± 0.02	-4.70
cyclopentene	-0.58 ± 0.00	1.96 ± 0.02	1.38 ± 0.02	0.56
cyclopropane	-0.03 ± 0.00	2.67 ± 0.02	2.64 ± 0.02	0.75
decan_1_ol	-5.16 ± 0.01	2.67 ± 0.03	-2.49 ± 0.03	-3.64
decan_2_one	-5.26 ± 0.01	3.28 ± 0.03	-1.98 ± 0.03	-2.34
di_isopropyl_sulfide	-2.56 ± 0.01	2.66 ± 0.02	0.10 ± 0.02	-1.21
di_n_butyl_ether	-2.65 ± 0.01	3.24 ± 0.03	0.59 ± 0.03	-0.83
di_n_butylamine	-4.71 ± 0.01	3.08 ± 0.03	-1.63 ± 0.03	-3.24
di_n_propyl_ether	-2.67 ± 0.01	2.88 ± 0.02	0.21 ± 0.02	-1.16
di_n_propyl_sulfide	-2.15 ± 0.01	2.64 ± 0.02	0.49 ± 0.02	-1.28
di_n_propylamine	-4.76 ± 0.01	2.50 ± 0.02	-2.26 ± 0.02	-3.65
dibromomethane	-1.10 ± 0.00	1.97 ± 0.02	0.87 ± 0.02	-1.96
dichloromethane	-1.60 ± 0.01	1.83 ± 0.01	0.23 ± 0.01	-1.31

diethoxymethoxybenzene	-7.19 ± 0.02	2.75 ± 0.03	-4.44 ± 0.04	-5.23
diethyl_disulfide	-2.51 ± 0.01	2.44 ± 0.02	-0.07 ± 0.02	-1.64
diethyl_ether	-3.02 ± 0.01	2.32 ± 0.02	-0.70 ± 0.02	-1.59
diethyl_malonate	-8.27 ± 0.02	1.82 ± 0.03	-6.45 ± 0.04	-6.00
diethyl_succinate	-10.32 ± 0.02	1.85 ± 0.03	-8.47 ± 0.04	-5.71
diethyl_sulfide	-2.18 ± 0.01	2.39 ± 0.02	0.21 ± 0.02	-1.46
diethylamine	-4.93 ± 0.01	2.21 ± 0.02	-2.72 ± 0.02	-4.07
diiodomethane	-2.30 ± 0.01	1.56 ± 0.02	-0.74 ± 0.02	-2.49
diisopropyl_ether	-3.01 ± 0.01	2.90 ± 0.02	-0.11 ± 0.02	-0.53
diisopropylamine	-4.60 ± 0.01	2.63 ± 0.02	-1.97 ± 0.02	-3.22
dimethoxymethane	-4.33 ± 0.01	1.64 ± 0.02	-2.69 ± 0.02	-2.93
dimethyl_disulfide	-0.72 ± 0.00	2.20 ± 0.02	1.48 ± 0.02	-1.83
dimethyl_ether	-2.70 ± 0.01	1.85 ± 0.02	-0.85 ± 0.02	-1.91
dimethyl_sulfate	-8.13 ± 0.01	0.28 ± 0.02	-7.85 ± 0.02	-5.10
dimethyl_sulfide	-1.70 ± 0.01	1.96 ± 0.02	0.26 ± 0.02	-1.61
dimethyl_sulfone	-11.21 ± 0.02	0.85 ± 0.02	-10.36 ± 0.03	-10.08
dimethyl_sulfoxide	-9.68 ± 0.02	1.36 ± 0.02	-8.32 ± 0.03	-8.71
dimethylamine	-4.72 ± 0.01	1.61 ± 0.02	-3.11 ± 0.02	-4.29
ethanamide	-9.94 ± 0.02	1.32 ± 0.02	-8.62 ± 0.03	-9.71
ethane	0.00 ± 0.00	2.58 ± 0.01	2.58 ± 0.01	1.83
ethanethiol	-2.49 ± 0.01	2.09 ± 0.02	-0.40 ± 0.02	-1.14
ethanol	-5.20 ± 0.02	1.75 ± 0.02	-3.45 ± 0.03	-5.00
ethene	-0.30 ± 0.00	2.66 ± 0.01	2.36 ± 0.01	1.28
ethyl_acetate	-5.14 ± 0.01	1.91 ± 0.02	-3.23 ± 0.02	-2.94
ethyl_benzoate	-6.33 ± 0.01	1.65 ± 0.02	-4.68 ± 0.02	-3.64
ethyl_butanoate	-5.39 ± 0.01	2.35 ± 0.02	-3.04 ± 0.02	-2.49
ethyl_formate	-4.52 ± 0.01	1.53 ± 0.02	-2.99 ± 0.02	-2.56
ethyl_hexanoate	-5.43 ± 0.02	2.63 ± 0.03	-2.80 ± 0.04	-2.23
ethyl_pentanoate	-5.47 ± 0.01	2.38 ± 0.03	-3.09 ± 0.03	-2.49
ethyl_phenyl_ether	-4.12 ± 0.01	2.11 ± 0.02	-2.01 ± 0.02	-2.22
ethyl_propanoate	-5.51 ± 0.01	2.12 ± 0.02	-3.39 ± 0.02	-2.68
ethylamine	-5.00 ± 0.01	1.86 ± 0.02	-3.14 ± 0.02	-4.50
ethylbenzene	-2.76 ± 0.01	2.17 ± 0.02	-0.59 ± 0.02	-0.79
fluorene	-5.31 ± 0.01	1.02 ± 0.02	-4.29 ± 0.02	-3.35
fluorobenzene	-2.10 ± 0.01	2.03 ± 0.02	-0.07 ± 0.02	-0.80
fluoromethane	-1.61 ± 0.01	2.40 ± 0.01	0.79 ± 0.01	-0.22
formaldehyde	-4.87 ± 0.01	1.65 ± 0.01	-3.22 ± 0.01	-2.75
halothane	-1.59 ± 0.01	2.29 ± 0.02	0.70 ± 0.02	-0.11
hept_1_ene	-0.33 ± 0.00	3.30 ± 0.02	2.97 ± 0.02	1.66
hept_1_yne	-0.80 ± 0.00	3.08 ± 0.02	2.28 ± 0.02	0.60
heptan_1_ol	-5.09 ± 0.01	2.37 ± 0.02	-2.72 ± 0.02	-4.21
heptan_2_one	-5.30 ± 0.01	2.50 ± 0.02	-2.80 ± 0.02	-3.04
heptan_4_one	-5.19 ± 0.01	2.51 ± 0.02	-2.68 ± 0.02	-2.92
heptanal	-5.06 ± 0.01	2.43 ± 0.03	-2.63 ± 0.03	-2.67
hex_1_ene	-0.33 ± 0.00	2.92 ± 0.02	2.59 ± 0.02	1.58
hex_1_yne	-0.81 ± 0.00	2.91 ± 0.02	2.10 ± 0.02	0.29
hexa_15_diene	-0.65 ± 0.01	3.09 ± 0.02	2.44 ± 0.02	1.01
hexafluoropropene	-1.17 ± 0.01	3.46 ± 0.02	2.29 ± 0.02	-3.76
hexan_1_ol	-5.08 ± 0.01	2.05 ± 0.02	-3.03 ± 0.02	-4.40
hexan_2_one	-5.28 ± 0.01	2.51 ± 0.02	-2.77 ± 0.02	-3.28
hexan_3_ol	-4.96 ± 0.01	2.33 ± 0.02	-2.63 ± 0.02	-4.06
hexanal	-5.09 ± 0.01	2.13 ± 0.02	-2.96 ± 0.02	-2.81
hexanoic_acid	-6.93 ± 0.02	1.85 ± 0.02	-5.08 ± 0.03	-6.21
hydrazine	-8.36 ± 0.02	1.26 ± 0.01	-7.10 ± 0.02	-9.30
hydrogen_sulfide	-3.05 ± 0.01	1.88 ± 0.01	-1.17 ± 0.01	-0.70
imidazole	-8.49 ± 0.02	0.64 ± 0.02	-7.85 ± 0.03	-9.63
indane	-2.97 ± 0.01	1.27 ± 0.02	-1.70 ± 0.02	-1.46
iodobenzene	-2.11 ± 0.01	1.77 ± 0.02	-0.34 ± 0.02	-1.74
iodoethane	-1.93 ± 0.01	1.83 ± 0.02	-0.10 ± 0.02	-0.74
iodomethane	-1.90 ± 0.01	1.93 ± 0.01	0.03 ± 0.01	-0.89
isoamyl_acetate	-5.44 ± 0.01	2.39 ± 0.03	-3.05 ± 0.03	-2.21

isoamyl_formate	-5.17 ± 0.01	1.78 ± 0.02	-3.39 ± 0.02	-2.13
isobutyl_acetate	-5.23 ± 0.01	2.43 ± 0.02	-2.80 ± 0.02	-2.36
isobutyl_formate	-5.00 ± 0.01	1.79 ± 0.02	-3.21 ± 0.02	-2.22
isobutyl_isobutanoate	-5.29 ± 0.01	2.74 ± 0.03	-2.55 ± 0.03	-1.69
isobutylbenzene	-2.66 ± 0.01	2.66 ± 0.02	0.00 ± 0.02	0.16
isobutyraldehyde	-4.98 ± 0.01	2.05 ± 0.02	-2.93 ± 0.02	-2.86
isoflurane	-4.21 ± 0.01	2.83 ± 0.02	-1.38 ± 0.02	0.10
isopropyl_acetate	-5.15 ± 0.02	2.23 ± 0.02	-2.92 ± 0.03	-2.64
isopropyl_formate	-4.37 ± 0.01	1.73 ± 0.02	-2.64 ± 0.02	-2.02
isopropylbenzene	-2.86 ± 0.01	2.55 ± 0.02	-0.31 ± 0.02	-0.30
m_bis_trifluoromethyl__benzene	-4.19 ± 0.01	2.61 ± 0.03	-1.58 ± 0.03	1.07
m_cresol	-6.94 ± 0.02	1.66 ± 0.02	-5.28 ± 0.03	-5.49
m_xylene	-2.71 ± 0.01	2.54 ± 0.02	-0.17 ± 0.02	-0.83
methane	0.00 ± 0.00	2.54 ± 0.01	2.54 ± 0.01	1.99
methanesulfonyl_chloride	-6.85 ± 0.01	0.52 ± 0.02	-6.33 ± 0.02	-4.87
methanethiol	-2.25 ± 0.01	1.99 ± 0.01	-0.26 ± 0.01	-1.24
methanol	-5.15 ± 0.01	1.67 ± 0.01	-3.48 ± 0.01	-5.10
methoxyflurane	-2.49 ± 0.01	1.78 ± 0.02	-0.71 ± 0.02	-1.12
methyl_acetate	-5.44 ± 0.01	1.71 ± 0.02	-3.73 ± 0.02	-3.13
methyl_benzoate	-6.30 ± 0.02	1.24 ± 0.02	-5.06 ± 0.03	-3.92
methyl_butanoate	-5.36 ± 0.01	2.04 ± 0.02	-3.32 ± 0.02	-2.83
methyl_chloroacetate	-5.16 ± 0.01	1.24 ± 0.02	-3.92 ± 0.02	-4.00
methyl_cyanoacetate	-6.89 ± 0.01	1.38 ± 0.02	-5.51 ± 0.02	-6.72
methyl_cyclohexanecarboxylate	-5.51 ± 0.01	1.22 ± 0.02	-4.29 ± 0.02	-3.30
methyl_cyclohexyl_ketone	-5.38 ± 0.01	1.48 ± 0.02	-3.90 ± 0.02	-3.90
methyl_cyclopropanecarboxylate	-6.30 ± 0.02	1.81 ± 0.03	-4.49 ± 0.04	-4.10
methyl_cyclopropyl_ketone	-5.82 ± 0.01	2.08 ± 0.02	-3.74 ± 0.02	-4.61
methyl_ethyl_ether	-2.84 ± 0.01	2.02 ± 0.02	-0.82 ± 0.02	-2.10
methyl_ethyl_sulfide	-1.93 ± 0.01	2.27 ± 0.02	0.34 ± 0.02	-1.50
methyl_formate	-4.48 ± 0.01	1.31 ± 0.02	-3.17 ± 0.02	-2.78
methyl_hexanoate	-5.36 ± 0.01	2.34 ± 0.03	-3.02 ± 0.03	-2.49
methyl_isopropyl_ether	-2.89 ± 0.01	2.14 ± 0.02	-0.75 ± 0.02	-2.01
methyl_methanesulfonate	-8.81 ± 0.02	0.52 ± 0.02	-8.29 ± 0.03	-4.87
methyl_octanoate	-5.31 ± 0.01	2.37 ± 0.03	-2.94 ± 0.03	-2.04
methyl_p_methoxybenzoate	-7.45 ± 0.01	1.13 ± 0.03	-6.32 ± 0.03	-5.33
methyl_p_nitrobenzoate	-6.27 ± 0.01	-0.12 ± 0.03	-6.39 ± 0.03	-6.88
methyl_pentanoate	-5.43 ± 0.01	1.92 ± 0.02	-3.51 ± 0.02	-2.56
methyl_propanoate	-5.47 ± 0.01	1.64 ± 0.02	-3.83 ± 0.02	-2.93
methyl_propyl_ether	-2.76 ± 0.01	2.35 ± 0.02	-0.41 ± 0.02	-1.66
methyl_t_butyl_ether	-2.95 ± 0.01	2.35 ± 0.02	-0.60 ± 0.02	-2.21
methyl_tert_butyl_ether	-2.90 ± 0.01	2.22 ± 0.02	-0.68 ± 0.02	-2.21
methyl_trifluoroacetate	-3.40 ± 0.01	2.01 ± 0.02	-1.39 ± 0.02	-1.10
methyl_trimethylacetate	-5.28 ± 0.01	2.29 ± 0.02	-2.99 ± 0.02	-2.40
methylamine	-5.13 ± 0.01	1.69 ± 0.01	-3.44 ± 0.01	-4.55
methylcyclohexane	0.01 ± 0.00	1.81 ± 0.02	1.82 ± 0.02	1.70
methylcyclopentane	0.00 ± 0.00	2.12 ± 0.02	2.12 ± 0.02	1.59
morpholine	-6.62 ± 0.01	0.34 ± 0.02	-6.28 ± 0.02	-7.17
n_butane	0.01 ± 0.00	2.53 ± 0.02	2.54 ± 0.02	2.07
n_butanethiol	-2.39 ± 0.01	2.27 ± 0.02	-0.12 ± 0.02	-0.99
n_butyl_acetate	-5.45 ± 0.01	2.28 ± 0.02	-3.17 ± 0.02	-2.64
n_butylacetamide	-9.76 ± 0.02	1.62 ± 0.02	-8.14 ± 0.03	-9.31
n_butylamine	-5.11 ± 0.01	2.29 ± 0.02	-2.82 ± 0.02	-4.24
n_butylbenzene	-2.76 ± 0.01	2.46 ± 0.02	-0.30 ± 0.02	-0.40
n_decane	0.01 ± 0.00	3.42 ± 0.03	3.43 ± 0.03	3.16
n_heptane	0.01 ± 0.00	3.19 ± 0.02	3.20 ± 0.02	2.67
n_heptylamine	-4.89 ± 0.01	2.17 ± 0.03	-2.72 ± 0.03	-3.79
n_hexane	0.01 ± 0.00	3.04 ± 0.02	3.05 ± 0.02	2.48
n_hexyl_acetate	-5.49 ± 0.01	2.52 ± 0.03	-2.97 ± 0.03	-2.26
n_hexylamine	-4.88 ± 0.01	2.34 ± 0.02	-2.54 ± 0.02	-3.95
n_hexylbenzene	-2.71 ± 0.01	2.95 ± 0.03	0.24 ± 0.03	-0.04
n_nonane	0.01 ± 0.00	3.31 ± 0.03	3.32 ± 0.03	3.13

n_octane	0.01 ± 0.00	3.12 ± 0.03	3.13 ± 0.03	2.88
n_octylamine	-5.12 ± 0.01	2.74 ± 0.03	-2.38 ± 0.03	-3.65
n_pentane	0.01 ± 0.00	2.66 ± 0.02	2.67 ± 0.02	2.32
n_pentyl_acetate	-5.40 ± 0.01	2.57 ± 0.03	-2.83 ± 0.03	-2.51
n_pentyl_propanoate	-5.96 ± 0.01	2.60 ± 0.03	-3.36 ± 0.03	-2.11
n_pentylamine	-5.12 ± 0.01	2.13 ± 0.02	-2.99 ± 0.02	-4.09
n_pentylbenzene	-2.75 ± 0.01	2.80 ± 0.03	0.05 ± 0.03	-0.23
n_pentylcyclopentane	0.00 ± 0.00	2.39 ± 0.03	2.39 ± 0.03	2.55
n_propanethiol	-2.41 ± 0.01	2.10 ± 0.02	-0.31 ± 0.02	-1.06
n_propyl_acetate	-5.30 ± 0.01	1.97 ± 0.02	-3.33 ± 0.02	-2.79
n_propyl_butyrate	-5.35 ± 0.01	2.47 ± 0.03	-2.88 ± 0.03	-2.28
n_propyl_formate	-5.03 ± 0.01	1.53 ± 0.02	-3.50 ± 0.02	-2.48
n_propyl_propanoate	-5.45 ± 0.01	2.50 ± 0.02	-2.95 ± 0.02	-2.44
n_propylamine	-4.83 ± 0.01	1.78 ± 0.02	-3.05 ± 0.02	-4.39
n_propylbenzene	-2.72 ± 0.01	2.73 ± 0.02	0.01 ± 0.02	-0.53
n_propylcyclopentane	0.00 ± 0.00	2.15 ± 0.02	2.15 ± 0.02	2.13
naphthalene	-4.51 ± 0.01	1.17 ± 0.02	-3.34 ± 0.02	-2.40
nitrobenzene	-3.63 ± 0.01	0.23 ± 0.02	-3.40 ± 0.02	-4.12
nitroethane	-2.47 ± 0.01	0.74 ± 0.02	-1.73 ± 0.02	-3.71
nitromethane	-2.53 ± 0.01	0.50 ± 0.01	-2.03 ± 0.01	-4.02
non_1_ene	-0.33 ± 0.00	3.24 ± 0.03	2.91 ± 0.03	2.06
nonan_1_ol	-5.10 ± 0.01	2.56 ± 0.03	-2.54 ± 0.03	-3.88
nonan_2_one	-5.29 ± 0.01	2.78 ± 0.03	-2.51 ± 0.03	-2.49
nonan_5_one	-5.20 ± 0.01	2.86 ± 0.03	-2.34 ± 0.03	-2.64
nonanal	-5.09 ± 0.01	2.58 ± 0.03	-2.51 ± 0.03	-2.07
o_cresol	-6.55 ± 0.01	1.46 ± 0.02	-5.09 ± 0.02	-5.87
o_toluidine	-6.81 ± 0.02	1.44 ± 0.02	-5.37 ± 0.03	-5.53
o_xylene	-2.75 ± 0.01	2.23 ± 0.02	-0.52 ± 0.02	-0.90
oct_1_ene	-0.33 ± 0.00	3.10 ± 0.03	2.77 ± 0.03	1.92
oct_1_yne	-0.83 ± 0.00	3.29 ± 0.02	2.46 ± 0.02	0.71
octan_1_ol	-5.13 ± 0.01	2.48 ± 0.03	-2.65 ± 0.03	-4.09
octan_2_one	-5.31 ± 0.01	3.01 ± 0.03	-2.30 ± 0.03	-2.88
octanal	-5.12 ± 0.01	2.55 ± 0.03	-2.57 ± 0.03	-2.29
p_cresol	-6.95 ± 0.01	1.59 ± 0.02	-5.36 ± 0.02	-6.13
p_dibromobenzene	-1.70 ± 0.01	1.69 ± 0.02	-0.01 ± 0.02	-2.30
p_toluidine	-6.91 ± 0.02	1.35 ± 0.02	-5.56 ± 0.03	-5.57
p_xylene	-2.71 ± 0.01	2.04 ± 0.02	-0.67 ± 0.02	-0.80
pent_1_ene	-0.34 ± 0.00	2.78 ± 0.02	2.44 ± 0.02	1.68
pent_1_yne	-0.81 ± 0.01	2.74 ± 0.02	1.93 ± 0.02	0.01
penta_14_diene	-0.70 ± 0.00	2.88 ± 0.02	2.18 ± 0.02	0.93
pentachloroethane	-1.13 ± 0.01	1.44 ± 0.02	0.31 ± 0.02	-1.39
pentan_1_ol	-5.13 ± 0.01	1.99 ± 0.02	-3.14 ± 0.02	-4.57
pentan_2_ol	-5.19 ± 0.01	2.32 ± 0.02	-2.87 ± 0.02	-4.39
pentan_2_one	-5.25 ± 0.01	1.96 ± 0.02	-3.29 ± 0.02	-3.52
pentan_3_ol	-4.89 ± 0.01	1.94 ± 0.02	-2.95 ± 0.02	-4.35
pentan_3_one	-5.23 ± 0.01	2.29 ± 0.02	-2.94 ± 0.02	-3.41
pentanal	-5.08 ± 0.01	2.12 ± 0.02	-2.96 ± 0.02	-3.03
pentanenitrile	-3.56 ± 0.01	2.32 ± 0.02	-1.24 ± 0.02	-3.52
pentanoic_acid	-7.01 ± 0.06	1.64 ± 0.02	-5.37 ± 0.06	-6.16
phenanthrene	-6.00 ± 0.01	0.85 ± 0.03	-5.15 ± 0.03	-3.88
phenol	-7.01 ± 0.02	1.34 ± 0.02	-5.67 ± 0.03	-6.61
phenyl_formate	-6.26 ± 0.01	1.43 ± 0.02	-4.83 ± 0.02	-3.82
phenyl_methyl_sulfide	-3.14 ± 0.01	1.93 ± 0.02	-1.21 ± 0.02	-2.73
phenyl_trifluoroethyl_ether	-5.49 ± 0.01	2.56 ± 0.02	-2.93 ± 0.02	-1.29
piperazine	-8.72 ± 0.02	0.38 ± 0.02	-8.34 ± 0.03	-7.40
piperidine	-4.68 ± 0.01	1.22 ± 0.02	-3.46 ± 0.02	-5.11
prop_2_en_1_ol	-5.18 ± 0.02	1.95 ± 0.02	-3.23 ± 0.03	-5.03
propan_1_ol	-5.10 ± 0.01	1.98 ± 0.02	-3.12 ± 0.02	-4.85
propan_2_ol	-5.29 ± 0.01	2.01 ± 0.02	-3.28 ± 0.02	-4.74
propane	0.00 ± 0.00	2.56 ± 0.02	2.56 ± 0.02	1.96
propanenitrile	-3.61 ± 0.01	2.34 ± 0.02	-1.27 ± 0.02	-3.84

propanoic_acid	-7.64 ± 0.02	1.23 ± 0.02	-6.41 ± 0.03	-6.46
propanone	-5.31 ± 0.01	1.95 ± 0.02	-3.36 ± 0.02	-3.80
propene	-0.37 ± 0.00	2.81 ± 0.02	2.44 ± 0.02	1.32
propionaldehyde	-5.06 ± 0.01	1.98 ± 0.02	-3.08 ± 0.02	-3.43
propyne	-0.87 ± 0.00	2.66 ± 0.02	1.79 ± 0.02	-0.48
pyrene	-7.03 ± 0.01	0.41 ± 0.03	-6.62 ± 0.03	-4.52
pyridine	-4.75 ± 0.01	1.30 ± 0.02	-3.45 ± 0.02	-4.69
pyrrole	-5.16 ± 0.01	1.29 ± 0.02	-3.87 ± 0.02	-4.78
pyrrolidine	-4.89 ± 0.01	0.98 ± 0.02	-3.91 ± 0.02	-5.48
quinoline	-5.70 ± 0.01	0.83 ± 0.02	-4.87 ± 0.02	-5.72
sec_butylbenzene	-2.72 ± 0.01	2.76 ± 0.03	0.04 ± 0.03	-0.45
styrene	-3.34 ± 0.01	2.02 ± 0.02	-1.32 ± 0.02	-1.24
teflurane	-1.99 ± 0.01	2.45 ± 0.02	0.46 ± 0.02	0.50
tert_butylbenzene	-2.98 ± 0.01	2.56 ± 0.03	-0.42 ± 0.03	-0.44
tetrachloroethene	-0.09 ± 0.00	1.50 ± 0.02	1.41 ± 0.02	0.10
tetrachloromethane	-0.13 ± 0.00	1.54 ± 0.02	1.41 ± 0.02	0.08
tetrafluoromethane	-0.38 ± 0.00	2.80 ± 0.01	2.42 ± 0.01	3.12
tetrahydrofuran	-3.30 ± 0.01	1.23 ± 0.02	-2.07 ± 0.02	-3.47
tetrahydropyran	-2.80 ± 0.01	1.02 ± 0.02	-1.78 ± 0.02	-3.12
thiophene	-1.88 ± 0.01	1.54 ± 0.02	-0.34 ± 0.02	-1.42
thiophenol	-3.26 ± 0.01	1.83 ± 0.02	-1.43 ± 0.02	-2.55
toluene	-2.70 ± 0.01	1.99 ± 0.02	-0.71 ± 0.02	-0.89
trans_14_dimethylcyclohexane	0.01 ± 0.00	2.04 ± 0.02	2.05 ± 0.02	2.11
triacetyl_glycerol	-13.83 ± 0.08	0.52 ± 0.03	-13.31 ± 0.08	-8.84
tribromomethane	-0.70 ± 0.00	1.58 ± 0.02	0.88 ± 0.02	-2.13
trichloroethene	-0.82 ± 0.00	1.81 ± 0.02	0.99 ± 0.02	-0.44
trichloromethane	-1.23 ± 0.00	1.55 ± 0.02	0.32 ± 0.02	-1.08
triethyl_phosphate	-11.94 ± 0.02	1.88 ± 0.03	-10.06 ± 0.04	-7.54
triethylamine	-4.28 ± 0.01	2.45 ± 0.03	-1.83 ± 0.03	-3.22
trimethoxy_methane	-5.97 ± 0.02	1.91 ± 0.02	-4.06 ± 0.03	-4.42
trimethoxymethylbenzene	-7.42 ± 0.02	1.59 ± 0.03	-5.83 ± 0.04	-4.04
trimethyl_phosphate	-11.33 ± 0.02	0.74 ± 0.02	-10.59 ± 0.03	-8.70
trimethylamine	-4.15 ± 0.01	1.83 ± 0.02	-2.32 ± 0.02	-3.20
undecan_2_one	-5.26 ± 0.01	3.14 ± 0.03	-2.12 ± 0.03	-2.15

Table 2 shows the same quantities as in Table 1, but only for those compounds affected by the amended Lennard-Jones well depth for triple bonded carbons. The revised results are shown.

TABLE 2:: Computed and experimental hydration free energies and components.

Molecule name	$\Delta G_{elec.}$	$\Delta G_{vdw.}$	$\Delta G_{hyd.}$	$\Delta G_{expt.}$
333_trimethoxypropionitrile	-6.93 ± 0.02	1.19 ± 0.03	-5.74 ± 0.04	-6.40
3_cyanophenol	-8.08 ± 0.02	1.09 ± 0.02	-6.99 ± 0.03	-9.65
3_cyanopyridine	-5.84 ± 0.01	1.21 ± 0.02	-4.63 ± 0.02	-6.75
4_cyanophenol	-8.65 ± 0.02	1.41 ± 0.02	-7.24 ± 0.03	-10.17
4_cyanopyridine	-6.01 ± 0.01	1.00 ± 0.02	-5.01 ± 0.02	-6.02
acetonitrile	-3.76 ± 0.01	1.25 ± 0.01	-2.51 ± 0.01	-3.88
benzonitrile	-4.14 ± 0.01	1.52 ± 0.02	-2.62 ± 0.02	-4.21
but_1_yne	-0.77 ± 0.01	1.28 ± 0.02	0.51 ± 0.02	-0.16
butanenitrile	-3.59 ± 0.01	1.36 ± 0.02	-2.23 ± 0.02	-3.64
cyanobenzene	-4.13 ± 0.01	1.57 ± 0.02	-2.56 ± 0.02	-4.10
hept_1_yne	-0.75 ± 0.00	1.59 ± 0.02	0.84 ± 0.02	0.60
hex_1_yne	-0.76 ± 0.00	1.55 ± 0.02	0.79 ± 0.02	0.29
methyl_cyanoacetate	-6.86 ± 0.01	0.52 ± 0.02	-6.34 ± 0.02	-6.72
oct_1_yne	-0.75 ± 0.00	1.87 ± 0.03	1.12 ± 0.03	0.71
pent_1_yne	-0.74 ± 0.00	1.19 ± 0.02	0.45 ± 0.02	0.01
pentanenitrile	-3.58 ± 0.01	1.42 ± 0.02	-2.16 ± 0.02	-3.52
propyne	-0.79 ± 0.00	0.99 ± 0.01	0.20 ± 0.01	-0.48

Table 3 shows the conversion between the names as tabulated in this work and IUPAC names (generated from the mol2 files using OpenEye's Lexichem package).

TABLE 3:: Names used for the tables and files here and the corresponding IUPAC names.

Test set name	IUPAC name
1112_tetrachloroethane	1,1,1,2-tetrachloroethane
111_trichloroethane	1,1,1-trichloroethane
111_trifluoro_222_trimethoxyethane	1,1,1-trifluoro-2,2,2-trimethoxy-ethane
111_trifluoropropan_2_ol	1,1,1-trifluoropropan-2-ol
111_trimethoxyethane	1,1,1-trimethoxyethane
1122_tetrachloroethane	1,1,2,2-tetrachloroethane
112_trichloro_122_trifluoroethane	1,1,2-trichloro-1,2,2-trifluoro-ethane
112_trichloroethane	1,1,2-trichloroethane
11_diacetoxyethane	1-acetoxyethyl acetate
11_dichloroethane	1,1-dichloroethane
11_dichloroethene	1,1-dichloroethylene
11_diethoxyethane	1,1-diethoxyethane
11_difluoroethane	1,1-difluoroethane
1234_tetrachlorobenzene	1,2,3,4-tetrachlorobenzene
1235_tetrachlorobenzene	1,2,3,5-tetrachlorobenzene
123_trichlorobenzene	1,2,3-trichlorobenzene
123_trimethylbenzene	1,2,3-trimethylbenzene
1245_tetrachlorobenzene	1,2,4,5-tetrachlorobenzene
124_trichlorobenzene	1,2,4-trichlorobenzene
124_trimethylbenzene	1,2,4-trimethylbenzene
12_diacetoxyethane	2-acetoxyethyl acetate
12_dibromoethane	1,2-dibromoethane
12_dichlorobenzene	1,2-dichlorobenzene
12_dichloroethane	1,2-dichloroethane
12_dichloropropane	1,2-dichloropropane
12_diethoxyethane	1,2-diethoxyethane
12_dimethoxyethane	1,2-dimethoxyethane
12_ethanediol	ethylene glycol
135_trichlorobenzene	1,3,5-trichlorobenzene
135_trimethylbenzene	mesitylene
13_dichlorobenzene	1,3-dichlorobenzene
13_dichloropropane	1,3-dichloropropane
13_dimethylnaphthalene	1,3-dimethylnaphthalene
14_dichlorobenzene	1,4-dichlorobenzene
14_dichlorobutane	1,4-dichlorobutane
14_dimethyl_piperazine	1,4-dimethylpiperazine
14_dimethylnaphthalene	1,4-dimethylnaphthalene
14_dioxane	1,4-dioxane
1_bromo_2_chloroethane	1-bromo-2-chloro-ethane
1_bromo_2_methylpropane	1-bromo-2-methyl-propane
1_bromobutane	1-bromobutane
1_bromoheptane	1-bromoheptane
1_bromohexane	1-bromohexane
1_bromooctane	1-bromooctane
1_bromopentane	1-bromopentane
1_bromopropane	1-bromopropane
1_chloro_222_trifluoroethane	2-chloro-1,1,1-trifluoro-ethane
1_chlorobutane	1-chlorobutane
1_chloroheptane	1-chloroheptane
1_chlorohexane	1-chlorohexane
1_chloropentane	1-chloropentane
1_chloropropane	1-chloropropane
1_ethylnaphthalene	1-ethylnaphthalene
1_iodobutane	1-iodobutane
1_iodoheptane	1-iodoheptane
1_iodohexane	1-iodohexane
1_iodopentane	1-iodopentane
1_iodopropane	1-iodopropane

1_methyl_imidazole	1-methylimidazole
1_methyl_pyrrole	1-methylpyrrole
1_methylcyclohexene	1-methylcyclohexene
1_methylnaphthalene	1-methylnaphthalene
1_naphthol	naphthalen-1-ol
1_naphthylamine	naphthalen-1-amine
1_nitrobutane	1-nitrobutane
1_nitropentane	1-nitropentane
1_nitropropane	1-nitropropane
222_trifluoroethanol	2,2,2-trifluoroethanol
224_trimethylpentane	2,2,4-trimethylpentane
225_trimethylhexane	2,2,5-trimethylhexane
22_dimethylbutane	2,2-dimethylbutane
22_dimethylpentane	2,2-dimethylpentane
22_dimethylpropane	neopentane
234_trimethylpentane	2,3,4-trimethylpentane
23_dimethylbuta_13_diene	2,3-dimethylbuta-1,3-diene
23_dimethylbutane	2,3-dimethylbutane
23_dimethylnaphthalene	2,3-dimethylnaphthalene
23_dimethylpentane	2,3-dimethylpentane
23_dimethylphenol	2,3-dimethylphenol
23_dimethylpyridine	2,3-dimethylpyridine
24_dimethylpentan_3_one	2,4-dimethylpentan-3-one
24_dimethylpentane	2,4-dimethylpentane
24_dimethylphenol	2,4-dimethylphenol
24_dimethylpyridine	2,4-dimethylpyridine
25_dimethylphenol	2,5-dimethylphenol
25_dimethylpyridine	2,5-dimethylpyridine
25_dimethyltetrahydrofuran	2,5-dimethyltetrahydrofuran
26_dimethylaniline	2,6-dimethylaniline
26_dimethylnaphthalene	2,6-dimethylnaphthalene
26_dimethylphenol	2,6-dimethylphenol
26_dimethylpyridine	2,6-dimethylpyridine
2_bromo_2_methylpropane	2-bromo-2-methyl-propane
2_bromopropane	2-bromopropane
2_butoxyethanol	2-butoxyethanol
2_chloro_111_trimethoxyethane	2-chloro-1,1,1-trimethoxy-ethane
2_chloro_2_methylpropane	2-chloro-2-methyl-propane
2_chloroaniline	2-chloroaniline
2_chlorobutane	2-chlorobutane
2_chlorophenol	2-chlorophenol
2_chloropropane	2-chloropropane
2_chloropyridine	2-chloropyridine
2_chlorotoluene	1-chloro-2-methyl-benzene
2_ethoxyethanol	2-ethoxyethanol
2_ethylpyrazine	2-ethylpyrazine
2_ethylpyridine	2-ethylpyridine
2_ethyltoluene	1-ethyl-2-methyl-benzene
2_fluorophenol	2-fluorophenol
2_iodophenol	2-iodophenol
2_iodopropane	2-iodopropane
2_isobutylpyrazine	2-isobutylpyrazine
2_methoxy_111_trimethoxyethane	1,1,1,2-tetramethoxyethane
2_methoxyaniline	2-methoxyaniline
2_methoxyethanamine	2-methoxyethanamine
2_methoxyethanol	2-methoxyethanol
2_methoxyphenol	2-methoxyphenol
2_methyl_but_2_ene	2-methylbut-2-ene
2_methylbut_2_ene	2-methylbut-2-ene
2_methylbuta_13_diene	isoprene
2_methylbutan_1_ol	2-methylbutan-1-ol

2_methylbutan_2_ol	2-methylbutan-2-ol
2_methylbutane	isopentane
2_methylhexane	2-methylhexane
2_methylpent_1_ene	2-methylpent-1-ene
2_methylpentan_2_ol	2-methylpentan-2-ol
2_methylpentan_3_ol	2-methylpentan-3-ol
2_methylpentane	isohexane
2_methylpropan_1_ol	2-methylpropan-1-ol
2_methylpropan_2_ol	2-methylpropan-2-ol
2_methylpropane	isobutane
2_methylpropene	2-methylprop-1-ene
2_methylpyrazine	2-methylpyrazine
2_methylpyridine	2-methylpyridine
2_methyltetrahydrofuran	2-methyltetrahydrofuran
2_methylthiophene	2-methylthiophene
2_naphthol	naphthalen-2-ol
2_naphthylamine	naphthalen-2-amine
2_nitroaniline	2-nitroaniline
2_nitrophenol	2-nitrophenol
2_nitropropane	2-nitropropane
2_nitrotoluene	1-methyl-2-nitro-benzene
2_phenylethanol	2-phenylethanol
2_propoxyethanol	2-propoxyethanol
333_trimethoxypropionitrile	3,3,3-trimethoxypropanenitrile
33_dimethylbutan_2_one	3,3-dimethylbutan-2-one
33_dimethylpentane	3,3-dimethylpentane
34_dimethylphenol	3,4-dimethylphenol
34_dimethylpyridine	3,4-dimethylpyridine
35_dimethylphenol	3,5-dimethylphenol
35_dimethylpyridine	3,5-dimethylpyridine
3_acetylpyridine	1-(3-pyridyl)ethanone
3_chloroaniline	3-chloroaniline
3_chlorophenol	3-chlorophenol
3_chloroprop_1_ene	3-chloroprop-1-ene
3_chloropyridine	3-chloropyridine
3_cyanophenol	3-hydroxybenzonitrile
3_cyanopyridine	pyridine-3-carbonitrile
3_ethylphenol	3-ethylphenol
3_ethylpyridine	3-ethylpyridine
3_formylpyridine	pyridine-3-carbaldehyde
3_hydroxybenzaldehyde	3-hydroxybenzaldehyde
3_methoxyaniline	3-methoxyaniline
3_methoxyphenol	3-methoxyphenol
3_methyl_1h_indole	3-methyl-1H-indole
3_methyl_but_1_ene	3-methylbut-1-ene
3_methylbut_1_ene	3-methylbut-1-ene
3_methylbutan_1_ol	3-methylbutan-1-ol
3_methylbutan_2_one	3-methylbutan-2-one
3_methylbutanoic_acid	3-methylbutanoic acid
3_methylheptane	3-methylheptane
3_methylhexane	3-methylhexane
3_methylpentane	3-methylpentane
3_methylpyridine	3-methylpyridine
3_nitroaniline	3-nitroaniline
3_nitrophenol	3-nitrophenol
3_nitrotoluene	1-methyl-3-nitro-benzene
3_phenylpropanol	3-phenylpropan-1-ol
4_acetylpyridine	1-(4-pyridyl)ethanone
4_bromophenol	4-bromophenol
4_bromotoluene	1-bromo-4-methyl-benzene
4_chloro_3_methylphenol	4-chloro-3-methyl-phenol

4_chloroaniline	4-chloroaniline
4_chlorophenol	4-chlorophenol
4_cyanophenol	4-hydroxybenzonitrile
4_cyanopyridine	pyridine-4-carbonitrile
4_ethylphenol	4-ethylphenol
4_ethylpyridine	4-ethylpyridine
4_ethyltoluene	1-ethyl-4-methyl-benzene
4_fluorophenol	4-fluorophenol
4_formylpyridine	pyridine-4-carbaldehyde
4_hydroxybenzaldehyde	4-hydroxybenzaldehyde
4_isopropyltoluene	1-isopropyl-4-methyl-benzene
4_methoxyacetophenone	1-(4-methoxyphenyl)ethanone
4_methoxyaniline	4-methoxyaniline
4_methyl_1h_imidazole	4-methyl-1H-imidazole
4_methylacetophenone	1-(p-tolyl)ethanone
4_methylbenzaldehyde	4-methylbenzaldehyde
4_methylpentan_2_ol	4-methylpentan-2-ol
4_methylpentan_2_one	4-methylpentan-2-one
4_methylpyridine	4-methylpyridine
4_n_propylphenol	4-propylphenol
4_nitroaniline	4-nitroaniline
4_nitrophenol	4-nitrophenol
4_tert_butylphenol	4-tert-butylphenol
E_12_dichloroethene	1,2-dichloroethylene
E_but_2_enal	but-2-enal
E_hept_2_ene	hept-2-ene
E_hex_2_enal	hex-2-enal
E_oct_2_enal	oct-2-enal
NN_dimethyl_p_methoxybenzamide	4-methoxy-N,N-dimethyl-benzamide
NN_dimethyl_p_methylbenzamide	N,N,4-trimethylbenzamide
NN_dimethyl_p_nitrobenzamide	N,N-dimethyl-4-nitro-benzamide
NN_dimethylaniline	N,N-dimethylaniline
NN_dimethylbenzamide	N,N-dimethylbenzamide
NN_dimethylformamide	N,N-dimethylformamide
N_acetylpyrrolidine	1-pyrrolidin-1-ylethanone
N_methyl_N__222_trifluoroethyl__aniline	N-methyl-N-(2,2,2-trifluoroethyl)aniline
N_methylacetamide	N-methylacetamide
N_methylaniline	N-methylaniline
N_methylmorpholine	4-methylmorpholine
N_methylpiperazine	1-methylpiperazine
N_methylpiperidine	1-methylpiperidine
Z_12_dichloroethene	1,2-dichloroethylene
Z_pent_2_ene	pent-2-ene
acenaphthene	acenaphthene
acetaldehyde	acetaldehyde
acetic_acid	acetic acid
acetonitrile	acetonitrile
acetophenone	1-phenylethanone
alpha_methylstyrene	isopropenylbenzene
ammonia	ammonia
aniline	aniline
anisole	anisole
anthracene	anthracene
azetidine	azetidine
benzaldehyde	benzaldehyde
benzamide	benzamide
benzene	benzene
benzonitrile	benzonitrile
benzotrifluoride	trifluoromethylbenzene
benzyl_alcohol	phenylmethanol
benzyl_bromide	bromomethylbenzene

benzyl_chloride	chloromethylbenzene
biphenyl	biphenyl
bis_2_chloroethyl__ether	1-chloro-2-(2-chloroethoxy)ethane
bromobenzene	bromobenzene
bromoethane	bromoethane
bromomethane	bromomethane
bromotrifluoromethane	bromo-trifluoro-methane
but_1_ene	but-1-ene
but_1_yne	but-1-yne
buta_13_diene	buta-1,3-diene
butan_1_ol	butan-1-ol
butan_2_ol	butan-2-ol
butanenitrile	butanenitrile
butanoic_acid	butyric acid
butanone	butanal
butyraldehyde	butanal
chlorobenzene	chlorobenzene
chlorodifluoromethane	chloro-difluoro-methane
chloroethane	chloroethane
chloroethylene	chloroethylene
chlorofluoromethane	chloro-fluoro-methane
chloromethane	chloromethane
cis_12_dimethylcyclohexane	1,2-dimethylcyclohexane
cyanobenzene	benzonitrile
cyclohepta_135_triene	cyclohepta-1,3,5-triene
cycloheptanol	cycloheptanol
cyclohexane	cyclohexane
cyclohexanol	cyclohexanol
cyclohexanone	cyclohexanone
cyclohexene	cyclohexene
cyclohexylamine	cyclohexanamine
cyclopentane	cyclopentane
cyclopentanol	cyclopentanol
cyclopentanone	cyclopentanone
cyclopentene	cyclopentene
cyclopropane	cyclopropane
decan_1_ol	decan-1-ol
decan_2_one	decan-2-one
di_isopropyl_sulfide	2-isopropylsulfanylpropane
di_n_butyl_ether	1-butoxybutane
di_n_butylamine	N-butylbutan-1-amine
di_n_propyl_ether	1-propoxypropane
di_n_propyl_sulfide	1-propylsulfanylpropane
di_n_propylamine	N-propylpropan-1-amine
dibromomethane	dibromomethane
dichloromethane	dichloromethane
diethoxymethoxybenzene	diethoxymethoxybenzene
diethyl_disulfide	ethyldisulfanylethane
diethyl_ether	ethoxyethane
diethyl_malonate	diethyl propanedioate
diethyl_succinate	diethyl butanedioate
diethyl_sulfide	ethylsulfanylethane
diethylamine	N-ethylethanamine
diiodomethane	diiodomethane
diisopropyl_ether	2-isopropoxypropane
diisopropylamine	N-isopropylpropan-2-amine
dimethoxymethane	dimethoxymethane
dimethyl_disulfide	methyldisulfanylmethane
dimethyl_ether	methoxymethane
dimethyl_sulfate	dimethyl sulfate
dimethyl_sulfide	methylsulfanylmethane

dimethyl_sulfone	methylsulfonylmethane
dimethyl_sulfoxide	methylsulfinylmethane
dimethylamine	N-methylmethanamine
ethanamide	acetamide
ethane	ethane
ethanethiol	ethanethiol
ethanol	ethanol
ethene	ethylene
ethyl_acetate	ethyl acetate
ethyl_benzoate	ethyl benzoate
ethyl_butanoate	ethyl butanoate
ethyl_formate	ethyl formate
ethyl_hexanoate	ethyl hexanoate
ethyl_pentanoate	ethyl pentanoate
ethyl_phenyl_ether	ethoxybenzene
ethyl_propanoate	ethyl propanoate
ethylamine	ethanamine
ethylbenzene	ethylbenzene
fluorene	9H-fluorene
fluorobenzene	fluorobenzene
fluoromethane	fluoromethane
formaldehyde	formaldehyde
halothane	2-bromo-2-chloro-1,1,1-trifluoro-ethane
hept_1_ene	hept-1-ene
hept_1_yne	hept-1-yne
heptan_1_ol	heptan-1-ol
heptan_2_one	heptan-2-one
heptan_4_one	heptan-4-one
heptanal	heptanal
hex_1_ene	hex-1-ene
hex_1_yne	hex-1-yne
hexa_15_diene	hexa-1,5-diene
hexafluoropropene	1,1,2,3,3,3-hexafluoroprop-1-ene
hexan_1_ol	hexan-1-ol
hexan_2_one	hexan-2-one
hexan_3_ol	hexan-3-ol
hexanal	hexanal
hexanoic_acid	hexanoic acid
hydrazine	hydrazine
hydrogen_sulfide	hydrogen sulfide
imidazole	imidazole
indane	indane
iodobenzene	iodobenzene
iodoethane	iodoethane
iodomethane	iodomethane
isoamyl_acetate	isopentyl acetate
isoamyl_formate	isopentyl formate
isobutyl_acetate	isobutyl acetate
isobutyl_formate	isobutyl formate
isobutyl_isobutanoate	isobutyl 2-methylpropanoate
isobutylbenzene	isobutylbenzene
isobutyraldehyde	2-methylpropanal
isoflurane	2-chloro-2-(difluoromethoxy)-1,1,1-trifluoro-ethane
isopropyl_acetate	isopropyl acetate
isopropyl_formate	isopropyl formate
isopropylbenzene	cumene
m_bis_trifluoromethyl__benzene	1,2-bis(trifluoromethyl)benzene
m_cresol	m-cresol
m_xylene	m-xylene
methane	methane
methanesulfonyl_chloride	methanesulfonyl chloride

methanethiol	methanethiol
methanol	methanol
methoxyflurane	2,2-dichloro-1,1-difluoro-1-methoxy-ethane
methyl_acetate	methyl acetate
methyl_benzoate	methyl benzoate
methyl_butanoate	methyl butanoate
methyl_chloroacetate	methyl 2-chloroacetate
methyl_cyanoacetate	methyl 2-cyanoacetate
methyl_cyclohexanecarboxylate	methyl cyclohexanecarboxylate
methyl_cyclohexyl_ketone	1-cyclohexylethanone
methyl_cyclopropanecarboxylate	methyl cyclopropanecarboxylate
methyl_cyclopropyl_ketone	1-cyclopropylethanone
methyl_ethyl_ether	methoxyethane
methyl_ethyl_sulfide	methylsulfanylethane
methyl_formate	methyl formate
methyl_hexanoate	methyl hexanoate
methyl_isopropyl_ether	2-methoxypropane
methyl_methanesulfonate	methyl methanesulfonate
methyl_octanoate	methyl octanoate
methyl_p_methoxybenzoate	methyl 4-methoxybenzoate
methyl_p_nitrobenzoate	methyl 4-nitrobenzoate
methyl_pentanoate	methyl pentanoate
methyl_propanoate	methyl propanoate
methyl_propyl_ether	1-methoxypropane
methyl_t_butyl_ether	2-methoxy-2-methyl-propane
methyl_tert_butyl_ether	2-methoxy-2-methyl-propane
methyl_trifluoroacetate	methyl 2,2,2-trifluoroacetate
methyl_trimethylacetate	methyl 2,2-dimethylpropanoate
methylamine	methanamine
methylcyclohexane	methylcyclohexane
methylcyclopentane	methylcyclopentane
morpholine	morpholine
n_butane	butane
n_butanethiol	butane-1-thiol
n_butyl_acetate	butyl acetate
n_butylacetamide	hexanamide
n_butylamine	butan-1-amine
n_butylbenzene	butylbenzene
n_decane	decane
n_heptane	heptane
n_heptylamine	heptan-1-amine
n_hexane	hexane
n_hexyl_acetate	hexyl acetate
n_hexylamine	hexan-1-amine
n_hexylbenzene	hexylbenzene
n_nonane	nonane
n_octane	octane
n_octylamine	octan-1-amine
n_pentane	pentane
n_pentyl_acetate	pentyl acetate
n_pentyl_propanoate	pentyl propanoate
n_pentylamine	pentan-1-amine
n_pentylbenzene	pentylbenzene
n_pentylcyclopentane	pentylcyclopentane
n_propanethiol	propane-1-thiol
n_propyl_acetate	propyl acetate
n_propyl_butyrate	propyl butanoate
n_propyl_formate	propyl formate
n_propyl_propanoate	propyl propanoate
n_propylamine	propan-1-amine
n_propylbenzene	propylbenzene

n_propylcyclopentane	propylcyclopentane
naphthalene	naphthalene
nitrobenzene	nitrobenzene
nitroethane	1-nitroethane
nitromethane	nitromethane
non_1_ene	non-1-ene
nonan_1_ol	nonan-1-ol
nonan_2_one	nonan-2-one
nonan_5_one	nonan-5-one
nonanal	nonanal
o_cresol	o-cresol
o_toluidine	2-methylaniline
o_xylene	o-xylene
oct_1_ene	oct-1-ene
oct_1_yne	oct-1-yne
octan_1_ol	octan-1-ol
octan_2_one	octan-2-one
octanal	octanal
p_cresol	p-cresol
p_dibromobenzene	1,4-dibromobenzene
p_toluidine	4-methylaniline
p_xylene	p-xylene
pent_1_ene	pent-1-ene
pent_1_yne	pent-1-yne
penta_14_diene	penta-1,4-diene
pentachloroethane	1,1,1,2,2-pentachloroethane
pentan_1_ol	pentan-1-ol
pentan_2_ol	pentan-2-ol
pentan_2_one	pentan-2-one
pentan_3_ol	pentan-3-ol
pentan_3_one	pentan-3-one
pentanal	pentanal
pentanenitrile	pentanenitrile
pentanoic_acid	pentanoic acid
phenanthrene	phenanthrene
phenol	phenol
phenyl_formate	phenyl formate
phenyl_methyl_sulfide	methylsulfanylbenzene
phenyl_trifluoroethyl_ether	1,2,2-trifluoroethoxybenzene
piperazine	piperazine
piperidine	piperidine
prop_2_en_1_ol	prop-2-en-1-ol
propan_1_ol	propan-1-ol
propan_2_ol	propan-2-ol
propane	propane
propanenitrile	propanenitrile
propanoic_acid	propionic acid
propanone	acetone
propene	prop-1-ene
propionaldehyde	propanal
propyne	prop-1-yne
pyrene	pyrene
pyridine	pyridine
pyrrole	pyrrole
pyrrolidine	pyrrolidine
quinoline	quinoline
sec_butylbenzene	sec-butylbenzene
styrene	styrene
teflurane	2-bromo-1,1,1,2-tetrafluoro-ethane
tert_butylbenzene	tert-butylbenzene
tetrachloroethene	1,1,2,2-tetrachloroethylene

tetrachloromethane	carbon tetrachloride
tetrafluoromethane	tetrafluoromethane
tetrahydrofuran	tetrahydrofuran
tetrahydropyran	tetrahydropyran
thiophene	thiophene
thiophenol	benzenethiol
toluene	toluene
trans_14_dimethylcyclohexane	1,4-dimethylcyclohexane
triacetyl_glycerol	3-acetyl-3,4-dihydroxy-4-(hydroxymethyl)hexane-2,5-dione
tribromomethane	bromoform
trichloroethene	1,1,2-trichloroethylene
trichloromethane	chloroform
triethyl_phosphate	triethyl phosphate
triethylamine	N,N-diethylethanamine
trimethoxy_methane	trimethoxymethane
trimethoxymethylbenzene	trimethoxymethylbenzene
trimethyl_phosphate	trimethyl phosphate
trimethylamine	N,N-dimethylmethanamine
undecan_2_one	undecan-2-one

Table 4 shows mean solvent accessible surface areas and volumes from simulations of the molecules in the test set.

TABLE 4:: Solvent accessible surface areas and volumes (angstrom units).

SASA	**SAV**
193.6 ± 0.1	234.8 ± 0.1
274.7 ± 0.4	364.6 ± 0.2
240.9 ± 0.1	307.3 ± 0.2
217.4 ± 0.1	272.0 ± 0.1
300.3 ± 0.2	396.7 ± 0.2
220.0 ± 0.1	279.0 ± 0.1
248.8 ± 0.1	323.5 ± 0.1
82.5 ± 0.0	69.6 ± 0.0
211.5 ± 0.1	266.0 ± 0.1
222.3 ± 0.1	283.1 ± 0.1
232.2 ± 0.2	286.4 ± 0.1
206.2 ± 0.1	253.8 ± 0.1
231.6 ± 0.1	294.2 ± 0.1
312.0 ± 0.3	408.3 ± 0.2
199.3 ± 0.1	242.0 ± 0.1
223.6 ± 0.2	284.9 ± 0.2
247.3 ± 0.2	324.3 ± 0.2
159.2 ± 0.1	179.7 ± 0.1
156.7 ± 0.1	173.7 ± 0.1
252.6 ± 0.2	321.3 ± 0.1
257.4 ± 0.2	343.8 ± 0.2
156.0 ± 0.1	174.7 ± 0.1
215.6 ± 0.1	266.4 ± 0.1
277.9 ± 0.3	359.0 ± 0.2
237.8 ± 0.1	306.3 ± 0.1
215.2 ± 0.1	264.8 ± 0.1
202.9 ± 0.1	247.7 ± 0.1
129.7 ± 0.1	136.5 ± 0.1
263.5 ± 0.2	349.0 ± 0.2
105.7 ± 0.0	102.2 ± 0.0
233.4 ± 0.1	287.8 ± 0.1
203.2 ± 0.1	247.4 ± 0.1
233.9 ± 0.1	300.3 ± 0.2
211.5 ± 0.1	265.9 ± 0.1
195.9 ± 0.1	232.4 ± 0.1
238.1 ± 0.1	302.4 ± 0.1
208.4 ± 0.1	255.7 ± 0.1

259.0 ± 0.2	338.9 ± 0.1
190.3 ± 0.1	225.6 ± 0.1
200.6 ± 0.1	247.3 ± 0.1
214.9 ± 0.1	266.2 ± 0.1
220.5 ± 0.1	273.3 ± 0.1
190.8 ± 0.1	228.6 ± 0.1
233.3 ± 0.2	298.2 ± 0.2
188.8 ± 0.1	219.5 ± 0.1
289.1 ± 0.2	400.0 ± 0.2
275.8 ± 0.1	376.3 ± 0.2
188.3 ± 0.1	224.7 ± 0.1
265.2 ± 0.1	353.9 ± 0.1
192.9 ± 0.1	230.7 ± 0.1
233.7 ± 0.1	298.6 ± 0.2
267.1 ± 0.2	358.4 ± 0.2
145.0 ± 0.1	156.9 ± 0.1
250.6 ± 0.2	326.5 ± 0.2
237.7 ± 0.1	306.6 ± 0.1
249.6 ± 0.2	321.6 ± 0.1
191.2 ± 0.1	226.5 ± 0.1
318.8 ± 0.1	449.5 ± 0.2
295.7 ± 0.2	401.0 ± 0.2
133.6 ± 0.1	141.8 ± 0.1
189.0 ± 0.1	222.1 ± 0.1
246.0 ± 0.2	328.1 ± 0.2
271.7 ± 0.2	361.8 ± 0.2
247.6 ± 0.2	322.3 ± 0.2
257.6 ± 0.3	324.8 ± 0.2
289.7 ± 0.2	396.3 ± 0.2
199.6 ± 0.1	238.7 ± 0.1
287.5 ± 0.2	371.1 ± 0.2
283.9 ± 0.3	367.2 ± 0.2
295.1 ± 0.2	400.4 ± 0.2
288.4 ± 0.3	386.5 ± 0.2
196.6 ± 0.1	244.4 ± 0.1
248.2 ± 0.2	319.6 ± 0.2
198.0 ± 0.1	233.6 ± 0.1
148.0 ± 0.1	157.9 ± 0.1
190.5 ± 0.1	224.7 ± 0.1
271.0 ± 0.2	371.6 ± 0.2
305.4 ± 0.3	433.9 ± 0.3
233.2 ± 0.2	287.6 ± 0.1
273.8 ± 0.3	343.9 ± 0.2
237.6 ± 0.1	303.9 ± 0.1
215.4 ± 0.1	258.4 ± 0.1
175.3 ± 0.1	201.7 ± 0.1
214.1 ± 0.1	266.7 ± 0.1
169.3 ± 0.1	194.0 ± 0.1
257.4 ± 0.2	325.0 ± 0.1
262.3 ± 0.2	335.1 ± 0.1
258.4 ± 0.2	330.1 ± 0.1
191.8 ± 0.1	234.6 ± 0.1
172.4 ± 0.1	198.1 ± 0.1
247.6 ± 0.1	326.7 ± 0.1
257.0 ± 0.1	333.6 ± 0.1
217.8 ± 0.1	274.3 ± 0.1
278.9 ± 0.6	356.0 ± 0.3
187.7 ± 0.1	221.0 ± 0.1
228.2 ± 0.2	283.0 ± 0.1
204.7 ± 0.1	255.8 ± 0.2
336.9 ± 0.5	460.8 ± 0.2

296.9 ± 0.2	415.9 ± 0.2
151.1 ± 0.1	165.9 ± 0.1
207.3 ± 0.1	257.1 ± 0.1
236.8 ± 0.1	303.9 ± 0.1
262.7 ± 0.3	337.3 ± 0.1
258.4 ± 0.2	329.3 ± 0.1
252.9 ± 0.2	327.4 ± 0.2
215.3 ± 0.3	263.6 ± 0.1
261.5 ± 0.2	346.8 ± 0.2
277.9 ± 0.2	357.8 ± 0.2
118.0 ± 0.0	117.9 ± 0.0
239.9 ± 0.2	301.0 ± 0.1
269.1 ± 0.1	358.3 ± 0.1
173.6 ± 0.1	196.4 ± 0.1
249.4 ± 0.3	313.7 ± 0.2
228.6 ± 0.1	290.6 ± 0.2
199.7 ± 0.1	239.9 ± 0.1
187.0 ± 0.1	228.9 ± 0.1
244.8 ± 0.1	314.9 ± 0.2
273.7 ± 0.2	359.8 ± 0.1
260.6 ± 0.2	329.1 ± 0.1
212.4 ± 0.1	269.7 ± 0.1
275.5 ± 0.2	361.9 ± 0.1
223.5 ± 0.2	284.7 ± 0.2
233.4 ± 0.2	300.4 ± 0.2
320.2 ± 0.2	445.1 ± 0.2
218.2 ± 0.1	275.7 ± 0.2
193.6 ± 0.1	227.0 ± 0.1
237.6 ± 0.1	304.0 ± 0.1
212.5 ± 0.1	264.5 ± 0.1
169.9 ± 0.1	194.5 ± 0.1
362.5 ± 0.3	494.9 ± 0.2
281.7 ± 0.7	381.6 ± 0.2
232.7 ± 0.2	297.8 ± 0.2
163.3 ± 0.1	183.8 ± 0.1
302.0 ± 0.3	392.1 ± 0.2
215.3 ± 0.1	271.3 ± 0.1
154.1 ± 0.1	171.1 ± 0.1
259.2 ± 0.2	337.3 ± 0.2
250.1 ± 0.2	326.0 ± 0.2
307.3 ± 0.4	400.5 ± 0.2
195.1 ± 0.1	242.0 ± 0.1
239.0 ± 0.1	306.3 ± 0.2
166.4 ± 0.1	189.0 ± 0.1
233.1 ± 0.1	298.9 ± 0.1
202.4 ± 0.1	241.6 ± 0.1
268.1 ± 0.2	340.3 ± 0.1
242.5 ± 0.1	323.1 ± 0.1
229.0 ± 0.1	292.7 ± 0.2
234.9 ± 0.1	302.5 ± 0.1
254.9 ± 0.2	326.7 ± 0.1
264.8 ± 0.2	338.3 ± 0.2
282.4 ± 0.3	362.0 ± 0.2
257.2 ± 0.1	342.5 ± 0.1
293.5 ± 0.1	393.1 ± 0.1
245.4 ± 0.2	322.7 ± 0.2
274.5 ± 0.2	381.7 ± 0.2
266.2 ± 0.2	344.0 ± 0.1
237.6 ± 0.1	302.5 ± 0.1
215.6 ± 0.2	268.0 ± 0.1
265.0 ± 0.2	333.4 ± 0.1

186.2 ± 0.1	227.9 ± 0.1
215.0 ± 0.1	263.6 ± 0.1
184.4 ± 0.1	216.5 ± 0.1
225.0 ± 0.1	288.7 ± 0.2
224.8 ± 0.3	280.2 ± 0.2
140.6 ± 0.1	150.9 ± 0.1
289.8 ± 0.3	376.1 ± 0.2
200.9 ± 0.1	245.9 ± 0.1
294.6 ± 0.2	382.0 ± 0.2
344.1 ± 0.4	456.9 ± 0.2
221.5 ± 0.1	275.7 ± 0.1
243.8 ± 0.2	319.8 ± 0.2
212.9 ± 0.1	256.2 ± 0.1
215.0 ± 0.1	270.6 ± 0.1
211.8 ± 0.2	262.3 ± 0.1
305.2 ± 0.3	395.4 ± 0.2
241.4 ± 0.2	320.6 ± 0.2
264.4 ± 0.2	349.3 ± 0.2
236.8 ± 0.1	303.5 ± 0.1
259.8 ± 0.1	346.5 ± 0.2
174.8 ± 0.1	196.7 ± 0.1
287.5 ± 0.4	371.3 ± 0.2
205.9 ± 0.1	245.5 ± 0.1
191.7 ± 0.1	225.2 ± 0.1
323.9 ± 0.2	442.0 ± 0.2
307.3 ± 0.7	399.6 ± 0.4
204.3 ± 0.1	243.1 ± 0.1
222.3 ± 0.1	275.7 ± 0.1
219.8 ± 0.1	275.8 ± 0.1
171.6 ± 0.1	202.3 ± 0.1
166.1 ± 0.1	188.7 ± 0.1
216.5 ± 0.1	267.5 ± 0.1
185.4 ± 0.1	215.0 ± 0.1
276.7 ± 0.1	365.3 ± 0.1
229.5 ± 0.2	286.2 ± 0.1
207.1 ± 0.1	260.2 ± 0.1
225.4 ± 0.1	289.5 ± 0.2
181.5 ± 0.1	210.4 ± 0.1
257.6 ± 0.2	324.5 ± 0.1
255.3 ± 0.1	334.1 ± 0.1
204.9 ± 0.1	251.6 ± 0.1
176.4 ± 0.1	210.3 ± 0.1
222.7 ± 0.2	273.3 ± 0.1
222.0 ± 0.2	270.6 ± 0.1
214.6 ± 0.1	258.2 ± 0.1
113.8 ± 0.0	112.7 ± 0.0
227.1 ± 0.2	284.5 ± 0.1
188.1 ± 0.1	229.0 ± 0.1
166.6 ± 0.1	189.3 ± 0.1
230.7 ± 0.1	294.9 ± 0.2
201.4 ± 0.1	248.4 ± 0.1
233.5 ± 0.1	291.7 ± 0.1
209.2 ± 0.1	264.4 ± 0.1
258.9 ± 0.2	350.4 ± 0.2
230.3 ± 0.1	292.9 ± 0.1
307.9 ± 0.2	419.6 ± 0.2
158.9 ± 0.1	175.6 ± 0.1
265.5 ± 0.1	353.7 ± 0.1
204.0 ± 0.2	246.0 ± 0.1
192.3 ± 0.2	230.4 ± 0.1
248.6 ± 0.2	326.8 ± 0.2

218.1 ± 0.1	274.6 ± 0.1
181.1 ± 0.1	219.4 ± 0.1
319.4 ± 0.2	433.6 ± 0.2
215.4 ± 0.2	263.1 ± 0.1
241.2 ± 0.1	307.6 ± 0.2
295.4 ± 0.2	408.6 ± 0.3
190.8 ± 0.1	227.7 ± 0.1
138.3 ± 0.1	147.9 ± 0.0
265.3 ± 0.2	349.7 ± 0.2
231.9 ± 0.1	300.0 ± 0.1
215.2 ± 0.1	272.0 ± 0.1
212.5 ± 0.2	258.5 ± 0.1
305.1 ± 0.2	399.4 ± 0.2
208.8 ± 0.1	257.3 ± 0.1
218.2 ± 0.1	270.3 ± 0.1
231.2 ± 0.1	295.5 ± 0.1
183.9 ± 0.1	224.0 ± 0.1
185.7 ± 0.1	218.6 ± 0.1
250.2 ± 0.1	323.4 ± 0.1
237.7 ± 0.2	296.0 ± 0.1
141.1 ± 0.1	151.5 ± 0.1
239.9 ± 0.2	295.7 ± 0.1
266.9 ± 0.1	338.5 ± 0.1
247.8 ± 0.2	308.6 ± 0.1
119.7 ± 0.0	120.9 ± 0.0
339.7 ± 0.5	451.1 ± 0.3
167.5 ± 0.1	187.8 ± 0.1
247.3 ± 0.1	314.9 ± 0.1
141.0 ± 0.1	149.8 ± 0.1
279.8 ± 0.1	355.8 ± 0.1
195.9 ± 0.1	229.4 ± 0.1
231.5 ± 0.1	286.3 ± 0.1
260.4 ± 0.2	352.9 ± 0.2
260.2 ± 0.2	351.0 ± 0.2
239.3 ± 0.1	309.7 ± 0.1
195.3 ± 0.1	233.9 ± 0.1
240.2 ± 0.3	301.2 ± 0.2
163.5 ± 0.1	185.6 ± 0.1
219.4 ± 0.1	283.0 ± 0.1
121.1 ± 0.1	121.9 ± 0.0
212.7 ± 0.1	261.8 ± 0.1
250.7 ± 0.1	328.7 ± 0.2
143.5 ± 0.0	156.3 ± 0.0
204.6 ± 0.1	248.8 ± 0.1
213.0 ± 0.1	261.7 ± 0.1
204.9 ± 0.1	256.8 ± 0.1
204.9 ± 0.1	247.9 ± 0.1
148.5 ± 0.1	165.7 ± 0.1
219.4 ± 0.1	265.6 ± 0.1
208.8 ± 0.1	250.3 ± 0.1
237.8 ± 0.7	302.3 ± 0.1
250.5 ± 0.1	326.5 ± 0.2
230.0 ± 0.1	289.3 ± 0.1
226.9 ± 0.2	290.4 ± 0.2
191.7 ± 0.1	225.8 ± 0.1
237.4 ± 0.1	306.0 ± 0.1
214.9 ± 0.2	263.3 ± 0.1
315.0 ± 0.3	413.6 ± 0.2
234.8 ± 0.1	302.5 ± 0.1
200.1 ± 0.1	242.7 ± 0.1
197.7 ± 0.1	235.8 ± 0.1

244.5 ± 0.1	317.0 ± 0.2
257.9 ± 0.3	324.9 ± 0.1
227.9 ± 0.1	291.6 ± 0.1
279.3 ± 0.2	361.1 ± 0.2
152.8 ± 0.1	168.0 ± 0.1
207.1 ± 0.1	249.4 ± 0.1
211.1 ± 0.1	271.4 ± 0.1
293.3 ± 0.2	407.7 ± 0.2
262.7 ± 0.2	333.7 ± 0.2
274.5 ± 0.5	364.2 ± 0.2
256.0 ± 0.1	320.9 ± 0.1
178.1 ± 0.1	207.3 ± 0.1
241.9 ± 0.1	312.1 ± 0.1
204.0 ± 0.1	249.3 ± 0.1
208.2 ± 0.1	249.8 ± 0.1
240.9 ± 0.2	312.7 ± 0.2
248.0 ± 0.1	317.8 ± 0.1
150.5 ± 0.1	164.0 ± 0.1
245.2 ± 0.1	315.4 ± 0.1
249.2 ± 0.2	318.9 ± 0.1
250.2 ± 0.2	337.3 ± 0.2
253.0 ± 0.2	317.7 ± 0.1
178.1 ± 0.1	208.0 ± 0.1
234.8 ± 0.2	297.3 ± 0.2
178.0 ± 0.1	208.1 ± 0.1
199.7 ± 0.1	245.8 ± 0.1
245.1 ± 0.2	320.5 ± 0.2
153.3 ± 0.1	167.7 ± 0.1
327.4 ± 0.2	426.4 ± 0.2
242.6 ± 0.1	305.9 ± 0.1
294.7 ± 0.2	406.9 ± 0.2
313.2 ± 0.4	424.0 ± 0.2
247.4 ± 0.2	323.8 ± 0.2
248.1 ± 0.1	318.5 ± 0.1
290.1 ± 0.4	380.4 ± 0.2
216.4 ± 0.1	263.0 ± 0.1
252.0 ± 0.4	324.9 ± 0.1
294.9 ± 0.2	408.2 ± 0.3
218.3 ± 0.1	273.0 ± 0.1
290.2 ± 0.2	387.0 ± 0.2
190.1 ± 0.1	224.7 ± 0.1
177.6 ± 0.1	204.2 ± 0.1
304.5 ± 0.2	404.9 ± 0.2
244.0 ± 0.1	318.2 ± 0.1
167.9 ± 0.1	191.7 ± 0.1
297.4 ± 0.2	385.8 ± 0.2
269.3 ± 0.2	357.2 ± 0.2
210.0 ± 0.1	264.3 ± 0.1
191.5 ± 0.1	223.4 ± 0.1
236.7 ± 0.1	303.3 ± 0.1
290.2 ± 0.3	376.1 ± 0.2
256.2 ± 0.1	338.9 ± 0.2
243.8 ± 0.1	315.0 ± 0.1
307.9 ± 0.3	435.4 ± 0.3
224.8 ± 0.1	291.0 ± 0.1
305.9 ± 0.6	399.1 ± 0.3
163.2 ± 0.1	183.5 ± 0.1
175.0 ± 0.1	199.1 ± 0.1
242.6 ± 0.1	317.6 ± 0.1
248.7 ± 0.1	325.8 ± 0.2
217.4 ± 0.1	271.9 ± 0.1

247.5 ± 0.1	314.0 ± 0.1
229.5 ± 0.1	300.5 ± 0.1
255.4 ± 0.3	324.3 ± 0.2
246.8 ± 0.1	321.1 ± 0.1
194.1 ± 0.1	233.4 ± 0.1
166.9 ± 0.1	188.3 ± 0.1
137.5 ± 0.1	145.4 ± 0.0
238.7 ± 0.1	304.3 ± 0.2
321.2 ± 1.2	427.3 ± 0.6
217.2 ± 0.3	267.9 ± 0.2
233.5 ± 0.2	299.2 ± 0.2
240.2 ± 0.1	312.5 ± 0.2
333.6 ± 0.3	442.1 ± 0.2
221.2 ± 0.1	266.6 ± 0.1
187.4 ± 0.1	222.4 ± 0.1
232.4 ± 0.2	286.8 ± 0.1
226.7 ± 0.2	289.7 ± 0.2
223.8 ± 0.1	284.7 ± 0.1
182.6 ± 0.1	212.1 ± 0.1
158.5 ± 0.1	177.1 ± 0.1
305.6 ± 0.2	409.4 ± 0.2
269.7 ± 0.2	344.5 ± 0.2
247.9 ± 0.1	317.4 ± 0.1
308.6 ± 0.3	404.6 ± 0.2
251.2 ± 0.2	326.7 ± 0.2
247.8 ± 0.1	321.0 ± 0.1
113.6 ± 0.0	113.6 ± 0.0
184.0 ± 0.1	217.0 ± 0.1
240.0 ± 0.2	302.2 ± 0.1
205.4 ± 0.1	254.3 ± 0.1
207.6 ± 0.1	252.0 ± 0.1
185.3 ± 0.1	220.0 ± 0.1
197.2 ± 0.1	236.6 ± 0.1
190.4 ± 0.1	227.3 ± 0.1
220.6 ± 0.1	281.3 ± 0.1
282.7 ± 0.4	362.4 ± 0.2
283.4 ± 0.2	382.4 ± 0.2
282.7 ± 0.3	362.6 ± 0.2
185.0 ± 0.1	217.9 ± 0.1
223.0 ± 0.1	286.7 ± 0.1
147.7 ± 0.1	160.7 ± 0.1
187.5 ± 0.1	221.6 ± 0.1
304.3 ± 0.4	393.5 ± 0.2
272.5 ± 0.3	348.3 ± 0.2
244.3 ± 0.2	306.7 ± 0.1
273.4 ± 0.3	362.8 ± 0.2
256.3 ± 0.2	340.5 ± 0.2
217.2 ± 0.1	268.0 ± 0.1
235.8 ± 0.1	303.0 ± 0.1
277.4 ± 0.1	368.1 ± 0.1
263.9 ± 0.2	345.1 ± 0.2
236.1 ± 0.1	300.3 ± 0.1
318.7 ± 0.4	464.5 ± 0.4
249.4 ± 0.2	325.7 ± 0.2
232.6 ± 0.1	297.7 ± 0.2
229.9 ± 0.1	296.0 ± 0.2
260.7 ± 0.2	346.8 ± 0.2
156.1 ± 0.1	172.2 ± 0.1
254.6 ± 0.2	338.4 ± 0.2
228.8 ± 0.2	284.6 ± 0.1
214.5 ± 0.1	259.5 ± 0.1

287.2 ± 0.3	372.5 ± 0.1
192.5 ± 0.1	239.2 ± 0.2
249.3 ± 0.1	310.9 ± 0.1
299.0 ± 0.3	411.2 ± 0.3
159.9 ± 0.1	182.9 ± 0.1
107.1 ± 0.1	99.1 ± 0.0
186.2 ± 0.1	221.4 ± 0.1
242.9 ± 0.1	312.3 ± 0.1
255.3 ± 0.2	323.1 ± 0.1
242.5 ± 0.1	315.1 ± 0.1
228.6 ± 0.1	293.8 ± 0.1
291.1 ± 0.2	375.6 ± 0.2
186.5 ± 0.1	220.2 ± 0.1
312.8 ± 0.4	412.6 ± 0.2
238.5 ± 0.1	304.0 ± 0.2
189.7 ± 0.1	223.0 ± 0.1
201.1 ± 0.1	246.0 ± 0.1
254.5 ± 0.3	323.8 ± 0.2
228.2 ± 0.1	288.1 ± 0.1
165.3 ± 0.1	191.0 ± 0.1
179.9 ± 0.1	211.3 ± 0.1
244.5 ± 0.2	316.1 ± 0.2
218.5 ± 0.1	268.7 ± 0.1
241.6 ± 0.2	300.8 ± 0.1
241.1 ± 0.1	313.6 ± 0.1
216.6 ± 0.2	275.9 ± 0.2
238.1 ± 0.2	296.6 ± 0.1
219.7 ± 0.2	269.4 ± 0.1
284.5 ± 0.2	383.1 ± 0.2
332.7 ± 0.3	437.4 ± 0.2
252.2 ± 0.2	317.5 ± 0.2
209.2 ± 0.2	254.8 ± 0.1
203.0 ± 0.1	247.3 ± 0.1
190.7 ± 0.1	226.5 ± 0.1
212.6 ± 0.1	271.9 ± 0.1
212.3 ± 0.2	259.9 ± 0.1
237.3 ± 0.2	297.4 ± 0.1
319.5 ± 0.3	419.4 ± 0.2
202.7 ± 0.1	245.5 ± 0.1
151.1 ± 0.1	165.4 ± 0.1
190.6 ± 0.1	226.3 ± 0.1
214.2 ± 0.1	270.4 ± 0.1
291.9 ± 0.2	406.1 ± 0.2
199.4 ± 0.1	250.5 ± 0.1
236.6 ± 0.2	307.1 ± 0.2
286.0 ± 0.1	390.1 ± 0.2
249.6 ± 0.2	326.6 ± 0.2
239.9 ± 0.1	310.4 ± 0.1
198.0 ± 0.1	242.9 ± 0.1
289.1 ± 0.2	383.0 ± 0.2
224.6 ± 0.1	284.3 ± 0.1
159.8 ± 0.1	179.8 ± 0.1
166.0 ± 0.1	189.1 ± 0.1
237.2 ± 0.2	309.9 ± 0.2
217.4 ± 0.1	274.6 ± 0.2
253.3 ± 0.2	320.5 ± 0.2
216.9 ± 0.1	274.6 ± 0.1
190.8 ± 0.1	228.9 ± 0.1
248.8 ± 0.2	323.5 ± 0.2
223.7 ± 0.1	283.7 ± 0.1
247.4 ± 0.2	310.7 ± 0.1

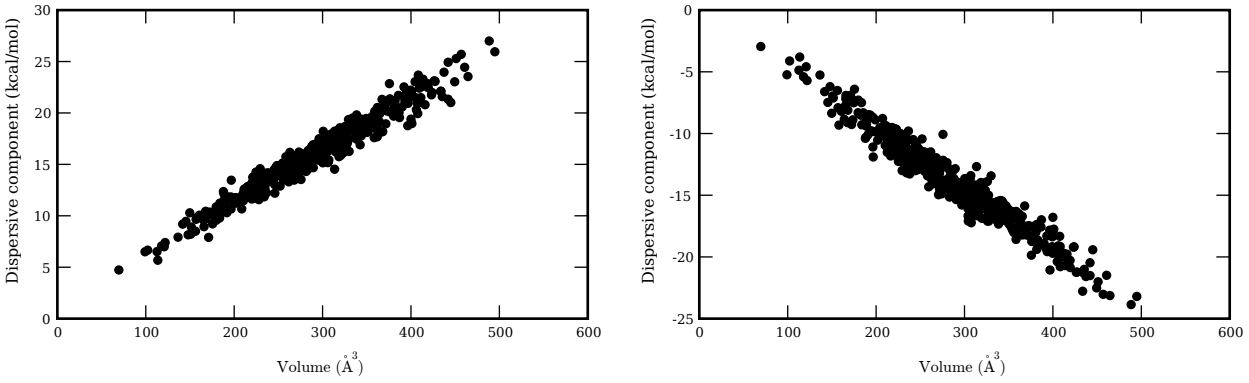
233.7 ± 0.2	299.5 ± 0.2
226.9 ± 0.1	289.8 ± 0.1
281.2 ± 0.4	361.8 ± 0.2
191.2 ± 0.1	233.4 ± 0.1
183.2 ± 0.1	212.1 ± 0.1
314.4 ± 0.5	413.2 ± 0.2
191.8 ± 0.1	229.9 ± 0.1
299.4 ± 0.3	394.9 ± 0.2
248.8 ± 0.1	327.2 ± 0.1
179.3 ± 0.1	208.5 ± 0.1
265.3 ± 0.3	338.9 ± 0.2
278.0 ± 0.2	363.1 ± 0.2
306.9 ± 0.2	423.2 ± 0.2
285.5 ± 0.2	379.9 ± 0.2
194.8 ± 0.1	232.0 ± 0.1
190.1 ± 0.1	232.0 ± 0.1
212.0 ± 0.1	266.2 ± 0.1
168.3 ± 0.1	193.6 ± 0.1
249.3 ± 0.2	325.5 ± 0.2
179.8 ± 0.1	211.2 ± 0.1
364.5 ± 0.8	488.5 ± 0.5
202.5 ± 0.1	252.7 ± 0.1
241.1 ± 0.2	312.9 ± 0.2
281.3 ± 0.2	381.4 ± 0.2
199.6 ± 0.1	238.0 ± 0.1
222.9 ± 0.2	285.0 ± 0.2
233.1 ± 0.1	300.9 ± 0.1
201.9 ± 0.1	254.9 ± 0.1
170.1 ± 0.1	196.5 ± 0.1
226.4 ± 0.2	291.0 ± 0.2
262.7 ± 0.2	354.3 ± 0.2
181.9 ± 0.1	215.3 ± 0.1
240.5 ± 0.1	314.9 ± 0.2
225.0 ± 0.2	276.6 ± 0.1
232.8 ± 0.1	298.3 ± 0.1
177.9 ± 0.1	212.6 ± 0.1
216.1 ± 0.1	271.7 ± 0.1
255.4 ± 0.1	337.2 ± 0.1
232.4 ± 0.1	297.0 ± 0.2
194.2 ± 0.1	238.6 ± 0.1

Input mol2 files with partial charges are available as a separate file in the supporting information, as are AMBER formatted parameter and coordinate files.

Table 5 shows the application of Student's *t*-test to comparing the calculated and experimental means by each functional group. For almost every functional group, the test indicates that the means are significantly different. This is not surprising since we observed a mean error of 0.676 ± 0.002 kcal/mol – solutes systematically prefer the gas phase too much relative to experiment.

Functional group	Number	*t*-value	Significance	Mean error
acid	73	2.47	0.02	-0.34
alcohol	38	-7.81	2e-09	1.29
aldehyde	20	0.53	0.6	-0.07
alkanes	28	-4.43	0.0001	0.31
alkene	35	-14.67	3e-16	1.07
alkyl bromide	17	-8.33	3e-07	1.50
alkyl chloride	31	-7.96	7e-09	1.09
alkyl iodide	9	-7.10	0.0001	0.86
alkyne	6	-7.17	0.0008	0.49
amine	44	-4.01	0.0002	0.55
aromatic compound	170	-6.86	1e-10	0.55
aryl chloride	20	-9.58	1e-08	1.04
carbonitrile	12	-7.11	2e-05	1.63
cyclic hydrocarbon	8	-2.26	0.06	0.21
ester	8	-0.04	1	0.02
ether	42	-7.58	3e-09	1.01
halogen derivative	22	-1.91	0.07	0.73
heterocyclic compound	48	-8.28	1e-10	1.02
hypervalent S	5	2.09	0.1	-1.50
ketone	25	-0.25	0.8	0.05
nitro compound	17	-4.91	0.0002	1.13
other	29	-1.74	0.09	0.55
phenol or hydroxyhetarene	33	-7.00	6e-08	1.16
thiol	5	-12.40	0.0002	0.89

TABLE 5: Statistics from applying Student's *t* test to the difference between the calculated and experimental means by funcational group. Shown are the number of compounds in each functional group, the calculated *t* value, the computed significance (probability that *t* could be this large or larger by chance) and the mean error for this group (in kcal/mol).



(a) Repulsive part of nonpolar component versus volume

(b) Attractive part of nonpolar component versus volume

Figure 1. Repulsive and attractive parts of the nonpolar component versus volume. Shown are the repulsive (a) and attractive (b) parts of the nonpolar component, as calculated using the WCA separation, plotted versus the solvent accessible volume for solutes in the test set. Similar plots comparing the repulsive and attractive components to surface area are given in the main text.