Comparative study on the gas to solution phase solvation free energies of model combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) in 178 organic solvents using the IEFPCM-UFF, CPCM, and SMD implicit solvent models at the Gaussian-4 (G4) level of theory

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Keywords: solvation free energy, combustion flue gas, organic solvents, Gaussian-4 (G4), implicit solvent models

Gas to solution phase standard state Gibbs free energies of solvation at 298.15 K (ΔG_s°) for transfer of six representative combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) were calculated at the Gaussian-4 (G4) level of theory using the IEFPCM-UFF, CPCM, and SMD implicit solvent models for 178 organic solvents. The IEFPCM-UFF and CPCM models yield similar ΔG_s° for all six compounds in each of the solvents considered, having maximum absolute intra-solvent deviations <1.6 kJ mol^{-1}. Substantial ΔG_s° differences were observed between the IEFPCM-UFF/CPCM and SMD models, with maximum absolute intra-solvent deviations up to 45.5 kJ mol^{-1}. The IEFPCM-UFF and CPCM models displayed strong ΔG_s° correlations with the solvent dielectric constant ($\varepsilon/\varepsilon_\circ$) for each compound, whereas the SMD model exhibits a significantly more variable ΔG_s° relationship with $\varepsilon/\varepsilon_\circ$.

Implicit solvation models are widely employed in theoretical studies to investigate the energetics of transferring molecules between gas, liquid, and solid phases, and for studying molecular structures, physical properties, and intra- and intermolecular reactions in the solution phase [1]. The majority of benchmarking efforts and applied studies using these types of solvent models are in aqueous solution, with generally more limited work conducted in a relatively small set of common organic solvents such as acetonitrile, dimethylsulfoxide, n-octanol, and methanol, among others (see, e.g., ref. [2–22], and references therein). A common property calculated by implicit solvation models is the gas to solution phase Gibbs free energy of solvation for small molecules, which is of value in calibrating/validating the theoretical models and of intrinsic interest for predicting partitioning behavior [23].

In the current work, the gas to solution phase Gibbs free energies of solvation at 1 mol L^{-1} concentration in each phase and 298.15 K (ΔG_s°) for transfer of six representative combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) were calculated at the Gaussian-4 (G4) [24] level of theory using the IEFPCM-UFF [25], CPCM [26,27], and SMD [19] implicit solvation models in Gaussian 09 [28] for all 178 single component organic solvents available within the self-consistent reaction field (SCRF) method of this software program, giving a total of 3204 individual data points (Tables 1 through 6). The compounds examined were chosen as di- and triatomic molecular proxies for the potential range of apolar/polar and aprotic/protic functional groups commonly present in larger organic compounds, and because the absolute and relative ΔG_s° of these molecules in organic solvents is relevant for assessing the carbon dioxide absorption capacity and separation selectivity from combustion flue gas streams [29–32]. Potential reactivity between the model compounds and solvents (e.g., CO_2 reacting with alcoholic, alkene, and amine solvents to form carbonates, carboxylic acids, and carbamates, respectively [30,32,33]) was not considered. In addition, the ΔG_s° values have utility where the thermodynamics of gas evolution and/or absorption is important for synthetic processes occurring in these solvents.

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Table 1. Calculated standard state (298.15 K, 1 mol L^{-1} → 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for dinitrogen (N_2) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-1.00	-1.02 [-0.02]	13.59 [14.60]
methanol	32.613	-1.00	-1.02 [-0.02]	12.62 [13.62]
ethanol	24.852	-0.98	-1.01 [-0.03]	12.90 [13.88]
isoquinoline	11	-0.90	-0.95 [-0.06]	7.20 [8.09]
quinoline	9.16	-0.87	-0.93 [-0.07]	7.24 [8.10]
chloroform	4.7113	-0.72	-0.82 [-0.11]	13.62 [14.33]
diethylether	4.24	-0.69	-0.80 [-0.11]	12.55 [13.23]
dichloromethane	8.93	-0.86	-0.93 [-0.07]	13.50 [14.37]
dichloroethane	10.125	-0.88	-0.95 [-0.06]	14.58 [15.47]
carbontetrachloride	2.228	-0.44	-0.57 [-0.13]	13.95 [14.39]
benzene	2.2706	-0.44	-0.58 [-0.13]	14.54 [14.98]
toluene	2.3741	-0.46	-0.60 [-0.13]	14.72 [15.18]
chlorobenzene	5.6968	-0.77	-0.86 [-0.09]	15.15 [15.92]
nitromethane	36.562	-1.01	-1.02 [-0.02]	14.92 [15.93]
heptane	1.9113	-0.36	-0.49 [-0.13]	13.67 [14.03]
cyclohexane	2.0165	-0.39	-0.52 [-0.13]	14.60 [14.99]
aniline	6.8882	-0.81	-0.90 [-0.08]	16.83 [17.64]
acetone	20.493	-0.97	-1.00 [-0.03]	13.09 [14.06]
tetrahydrofuran	7.4257	-0.83	-0.91 [-0.08]	14.18 [15.01]
dimethylsulfoxide	46.826	-1.02	-1.03 [-0.01]	16.03 [17.05]
n-octanol	9.8629	-0.88	-0.94 [-0.06]	14.27 [15.15]
1,1,1-trichloroethane	7.0826	-0.82	-0.90 [-0.08]	13.56 [14.38]
1,1,2-trichloroethane	7.1937	-0.82	-0.90 [-0.08]	14.98 [15.81]
1,2,4-trimethylbenzene	2.3653	-0.46	-0.60 [-0.13]	15.26 [15.73]
1,2-dibromoethane	4.9313	-0.73	-0.83 [-0.10]	16.57 [17.30]
1,2-ethanediol	40.245	-1.01	-1.03 [-0.02]	16.82 [17.83]
1,4-dioxane	2.2099	-0.43	-0.56 [-0.13]	15.56 [15.99]
1-bromo-2-methylpropane	7.7792	-0.84	-0.91 [-0.07]	13.92 [14.76]
1-bromooctane	5.0244	-0.74	-0.83 [-0.10]	14.85 [15.58]
1-bromopentane	6.269	-0.79	-0.88 [-0.09]	14.45 [15.24]
1-bromopropane	8.0496	-0.85	-0.92 [-0.07]	14.02 [14.87]
1-butanol	17.332	-0.95	-0.99 [-0.04]	13.64 [14.60]
1-chlorohexane	5.9491	-0.78	-0.87 [-0.09]	14.12 [14.90]
1-chloropentane	6.5022	-0.80	-0.88 [-0.08]	13.85 [14.65]
1-chloropropane	8.3548	-0.85	-0.92 [-0.07]	13.11 [13.96]
1-decanol	7.5305	-0.83	-0.91 [-0.08]	14.59 [15.42]
1-fluorooctane	3.89	-0.66	-0.77 [-0.12]	13.80 [14.46]
1-heptanol	11.321	-0.90	-0.96 [-0.06]	14.16 [15.06]
1-hexanol	12.51	-0.92	-0.97 [-0.05]	13.96 [14.88]
1-hexene	2.0717	-0.40	-0.53 [-0.13]	13.35 [13.76]
1-hexyne	2.615	-0.51	-0.64 [-0.13]	13.61 [14.11]
1-iodobutane	6.173	-0.79	-0.88 [-0.09]	15.14 [15.93]
1-iodohexadecane	3.5338	-0.62	-0.75 [-0.12]	15.72 [16.35]
1-iodopentane	5.6973	-0.77	-0.86 [-0.09]	15.21 [15.98]
1-iodopropane	6.9626	-0.82	-0.90 [-0.08]	15.22 [16.04]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-0.98	-1.01 [-0.03]	14.30 [15.28]
1-nonanol	8.5991	-0.86	-0.93 [-0.07]	14.44 [15.30]
1-pentanol	15.13	-0.94	-0.98 [-0.04]	13.81 [14.75]
1-pentene	1.9905	-0.38	-0.51 [-0.13]	12.96 [13.34]
1-propanol	20.524	-0.97	-1.00 [-0.03]	13.30 [14.26]
2,2,2-trifluoroethanol	26.726	-0.99	-1.01 [-0.03]	12.81 [13.80]
2,2,4-trimethylpentane	1.9358	-0.37	-0.50 [-0.13]	13.52 [13.89]
2,4-dimethylpentane	1.8939	-0.36	-0.48 [-0.13]	13.36 [13.72]
2,4-dimethylpyridine	9.4176	-0.87	-0.94 [-0.07]	15.17 [16.04]
2,6-dimethylpyridine	7.1735	-0.82	-0.90 [-0.08]	14.99 [15.81]
2-bromopropane	9.361	-0.87	-0.93 [-0.06]	13.64 [14.52]
2-butanol	15.944	-0.94	-0.98 [-0.04]	13.33 [14.28]
2-chlorobutane	8.393	-0.85	-0.92 [-0.07]	13.26 [14.12]
2-heptanone	11.658	-0.91	-0.96 [-0.05]	13.94 [14.85]
2-hexanone	14.136	-0.93	-0.98 [-0.05]	13.75 [14.68]
2-methoxyethanol	17.2	-0.95	-0.99 [-0.04]	14.44 [15.39]
2-methyl-1-propanol	16.777	-0.95	-0.99 [-0.04]	13.30 [14.25]
2-methyl-2-propanol	12.47	-0.91	-0.97 [-0.05]	12.96 [13.87]
2-methylpentane	1.89	-0.36	-0.48 [-0.13]	13.18 [13.54]
2-methylpyridine	9.9533	-0.88	-0.94 [-0.06]	15.04 [15.92]
2-nitropropane	25.654	-0.98	-1.01 [-0.03]	14.12 [15.11]
2-octanone	9.4678	-0.87	-0.94 [-0.06]	14.01 [14.88]
2-pentanone	15.2	-0.94	-0.98 [-0.04]	13.36 [14.30]
2-propanol	19.264	-0.96	-1.00 [-0.03]	12.93 [13.89]
2-propen-1-ol	19.011	-0.96	-1.00 [-0.03]	13.80 [14.76]
3-methylpyridine	11.645	-0.91	-0.96 [-0.05]	15.27 [16.17]
3-pentanone	16.78	-0.95	-0.99 [-0.04]	13.57 [14.51]
4-heptanone	12.257	-0.91	-0.96 [-0.05]	13.77 [14.68]
4-methyl-2-pentanone	12.887	-0.92	-0.97 [-0.05]	13.48 [14.40]
4-methylpyridine	11.957	-0.91	-0.96 [-0.05]	15.31 [16.22]
5-nonanone	10.6	-0.89	-0.95 [-0.06]	14.07 [14.96]
aceticacid	6.2528	-0.79	-0.88 [-0.09]	13.92 [14.71]
acetophenone	17.44	-0.95	-0.99 [-0.04]	16.14 [17.09]
2-chlorotoluene	6.7175	-0.81	-0.89 [-0.08]	15.92 [16.73]
anisole	4.2247	-0.69	-0.80 [-0.11]	15.71 [16.39]
benzaldehyde	18.22	-0.96	-0.99 [-0.04]	15.77 [16.72]
benzonitrile	25.592	-0.98	-1.01 [-0.03]	15.87 [16.86]
benzylalcohol	12.457	-0.91	-0.97 [-0.05]	15.80 [16.71]
bromobenzene	5.3954	-0.75	-0.85 [-0.10]	15.76 [16.52]
bromoethane	9.01	-0.87	-0.93 [-0.07]	13.61 [14.47]
bromoform	4.2488	-0.69	-0.80 [-0.11]	17.30 [17.99]
butanal	13.45	-0.92	-0.97 [-0.05]	13.48 [14.41]
butanoicacid	2.9931	-0.56	-0.69 [-0.13]	14.31 [14.87]
butanone	18.246	-0.96	-0.99 [-0.04]	13.34 [14.30]
butanonitrile	24.291	-0.98	-1.01 [-0.03]	13.74 [14.72]
butylamine	4.6178	-0.71	-0.82 [-0.11]	13.81 [14.52]
butylethanoate	4.9941	-0.73	-0.83 [-0.10]	13.89 [14.62]
carbondisulfide	2.6105	-0.51	-0.64 [-0.13]	17.06 [17.56]
cis-1,2-dimethylcyclohexane	2.06	-0.40	-0.53 [-0.13]	14.74 [15.14]
cis-decalin	2.2139	-0.43	-0.56 [-0.13]	15.89 [16.33]
cyclohexanone	15.619	-0.94	-0.98 [-0.04]	15.34 [16.28]

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solvent	$\varepsilon/\varepsilon_o$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-0.38	-0.50 [-0.13]	14.09 [14.47]
cyclopentanol	16.989	-0.95	-0.99 [-0.04]	15.08 [16.03]
cyclopentanone	13.58	-0.92	-0.97 [-0.05]	15.01 [15.93]
dibromomethane	7.2273	-0.82	-0.90 [-0.08]	16.08 [16.90]
dibutylether	3.0473	-0.57	-0.70 [-0.13]	14.17 [14.74]
diethylamine	3.5766	-0.63	-0.75 [-0.12]	13.32 [13.95]
diethylsulfide	5.723	-0.77	-0.86 [-0.09]	14.21 [14.98]
diiodomethane	5.32	-0.75	-0.85 [-0.10]	22.12 [22.87]
diisopropylether	3.38	-0.61	-0.73 [-0.12]	12.86 [13.47]
dimethyldisulfide	9.6	-0.88	-0.94 [-0.06]	15.93 [16.80]
diphenylether	3.73	-0.64	-0.76 [-0.12]	14.88 [15.53]
dipropylamine	2.9112	-0.55	-0.68 [-0.13]	13.90 [14.45]
E-1,2-dichloroethene	2.14	-0.42	-0.55 [-0.13]	14.44 [14.86]
E-2-pentene	2.051	-0.40	-0.53 [-0.13]	13.13 [13.53]
ethanethiol	6.667	-0.81	-0.89 [-0.08]	13.87 [14.68]
ethylbenzene	2.4339	-0.48	-0.61 [-0.13]	14.99 [15.46]
ethylethanoate	5.9867	-0.78	-0.87 [-0.09]	13.45 [14.23]
ethylmethanoate	8.331	-0.85	-0.92 [-0.07]	13.22 [14.08]
ethylphenylether	4.1797	-0.68	-0.79 [-0.11]	15.41 [16.09]
fluorobenzene	5.42	-0.76	-0.85 [-0.09]	13.89 [14.65]
formamide	108.94	-1.04	-1.04 [-0.01]	18.08 [19.11]
formicacid	51.1	-1.02	-1.03 [-0.01]	14.90 [15.92]
hexanoicacid	2.6	-0.50	-0.64 [-0.13]	14.73 [15.24]
iodobenzene	4.547	-0.71	-0.81 [-0.11]	16.82 [17.52]
iodoethane	7.6177	-0.83	-0.91 [-0.07]	15.21 [16.05]
iodomethane	6.865	-0.81	-0.89 [-0.08]	15.70 [16.51]
isopropylbenzene	2.3712	-0.46	-0.60 [-0.13]	14.96 [15.42]
m-cresol	12.44	-0.91	-0.97 [-0.05]	15.69 [16.60]
mesitylene	2.265	-0.44	-0.57 [-0.13]	15.03 [15.48]
methylbenzoate	6.7367	-0.81	-0.89 [-0.08]	16.02 [16.82]
methylbutanoate	5.5607	-0.76	-0.86 [-0.09]	13.77 [14.53]
methylcyclohexane	2.024	-0.39	-0.52 [-0.13]	14.40 [14.79]
methylethanoate	6.8615	-0.81	-0.89 [-0.08]	13.49 [14.30]
methylmethanoate	8.8377	-0.86	-0.93 [-0.07]	13.22 [14.09]
methylpropanoate	6.0777	-0.79	-0.87 [-0.09]	13.63 [14.41]
m-xylene	2.3478	-0.46	-0.59 [-0.13]	14.99 [15.45]
n-butylbenzene	2.36	-0.46	-0.59 [-0.13]	15.17 [15.63]
n-decane	1.9846	-0.38	-0.51 [-0.13]	14.31 [14.69]
n-dodecane	2.006	-0.39	-0.51 [-0.13]	14.60 [14.98]
n-hexadecane	2.0402	-0.39	-0.53 [-0.13]	14.97 [15.36]
n-hexane	1.8819	-0.35	-0.48 [-0.13]	13.34 [13.70]
nitrobenzene	34.809	-1.00	-1.02 [-0.02]	16.35 [17.36]
nitroethane	28.29	-0.99	-1.01 [-0.02]	14.46 [15.45]
N-methylaniline	5.96	-0.78	-0.87 [-0.09]	16.24 [17.02]
N,N-dimethylacetamide	37.781	-1.01	-1.02 [-0.02]	14.95 [15.95]
N,N-dimethylformamide	37.219	-1.01	-1.02 [-0.02]	15.06 [16.07]
n-nonane	1.9605	-0.38	-0.50 [-0.13]	14.15 [14.52]
n-octane	1.9406	-0.37	-0.50 [-0.13]	13.93 [14.30]
n-pentadecane	2.0333	-0.39	-0.52 [-0.13]	14.89 [15.29]
n-pentane	1.8371	-0.34	-0.47 [-0.13]	12.90 [13.25]
n-undecane	1.991	-0.38	-0.51 [-0.13]	14.66 [15.04]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-0.71	-0.82 [-0.11]	15.44 [16.15]
o-cresol	6.76	-0.81	-0.89 [-0.08]	15.93 [16.74]
o-dichlorobenzene	9.9949	-0.88	-0.94 [-0.06]	15.81 [16.70]
o-nitrotoluene	25.669	-0.98	-1.01 [-0.03]	16.52 [17.50]
o-xylene	2.5454	-0.50	-0.63 [-0.13]	15.17 [15.67]
pentanal	10	-0.88	-0.94 [-0.06]	13.76 [14.65]
pentanoicacid	2.6924	-0.52	-0.65 [-0.13]	14.53 [15.05]
pentylamine	4.201	-0.68	-0.79 [-0.11]	14.39 [15.07]
pentylethanoate	4.7297	-0.72	-0.82 [-0.10]	14.02 [14.74]
perfluorobenzene	2.029	-0.39	-0.52 [-0.13]	13.16 [13.55]
p-isopropyltoluene	2.2322	-0.44	-0.57 [-0.13]	14.94 [15.38]
propanal	18.5	-0.96	-1.00 [-0.04]	13.03 [13.99]
propanoicacid	3.44	-0.61	-0.74 [-0.12]	14.16 [14.78]
propanonitrile	29.324	-0.99	-1.02 [-0.02]	13.54 [14.53]
propylamine	4.9912	-0.73	-0.83 [-0.10]	13.43 [14.16]
propylethanoate	5.5205	-0.76	-0.86 [-0.09]	13.63 [14.40]
p-xylene	2.2705	-0.44	-0.58 [-0.13]	14.94 [15.38]
pyridine	12.978	-0.92	-0.97 [-0.05]	15.37 [16.29]
sec-butylbenzene	2.3446	-0.46	-0.59 [-0.13]	15.08 [15.54]
tert-butylbenzene	2.3447	-0.46	-0.59 [-0.13]	15.06 [15.52]
tetrachloroethene	2.268	-0.44	-0.57 [-0.13]	15.30 [15.74]
tetrahydrothiophene-S,S-dioxide	43.962	-1.01	-1.03 [-0.02]	18.90 [19.91]
tetralin	2.771	-0.53	-0.66 [-0.13]	16.08 [16.61]
thiophene	2.727	-0.53	-0.65 [-0.13]	15.36 [15.89]
thiophenol	4.2728	-0.69	-0.80 [-0.11]	16.54 [17.23]
trans-decalin	2.1781	-0.43	-0.56 [-0.13]	15.51 [15.94]
tributylphosphate	8.1781	-0.85	-0.92 [-0.07]	13.23 [14.08]
trichloroethene	3.422	-0.61	-0.74 [-0.12]	14.64 [15.25]
triethylamine	2.3832	-0.47	-0.60 [-0.13]	13.71 [14.18]
xylenemixture	2.3879	-0.47	-0.60 [-0.13]	15.03 [15.50]
Z-1,2-dichloroethene	9.2	-0.87	-0.93 [-0.07]	14.10 [14.97]

Table 2. Calculated standard state (298.15 K, 1 mol L^{-1} → 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for carbon dioxide (CO_2) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-6.01	-6.11 [-0.09]	-0.42 [5.59]
methanol	32.613	-5.99	-6.09 [-0.10]	15.66 [21.65]
ethanol	24.852	-5.89	-6.02 [-0.13]	11.89 [17.78]
isoquinoline	11	-5.41	-5.68 [-0.27]	-4.91 [0.50]
quinoline	9.16	-5.25	-5.56 [-0.32]	-4.76 [0.49]
chloroform	4.7113	-4.37	-4.88 [-0.51]	5.52 [9.89]
diethylether	4.24	-4.18	-4.72 [-0.54]	-3.98 [0.20]
dichloromethane	8.93	-5.22	-5.54 [-0.32]	2.29 [7.51]
dichloroethane	10.125	-5.34	-5.63 [-0.29]	2.90 [8.24]
carbontetrachloride	2.228	-2.70	-3.35 [-0.65]	0.06 [2.76]
benzene	2.2706	-2.75	-3.40 [-0.65]	-0.60 [2.15]
toluene	2.3741	-2.87	-3.53 [-0.65]	-0.39 [2.49]
chlorobenzene	5.6968	-4.67	-5.12 [-0.45]	-0.69 [3.98]
nitromethane	36.562	-6.02	-6.11 [-0.09]	0.53 [6.55]
heptane	1.9113	-2.25	-2.88 [-0.63]	0.72 [2.97]
cyclohexane	2.0165	-2.41	-3.05 [-0.64]	1.38 [3.79]
aniline	6.8882	-4.93	-5.32 [-0.39]	10.13 [15.05]
acetone	20.493	-5.81	-5.97 [-0.15]	-3.28 [2.53]
tetrahydrofuran	7.4257	-5.02	-5.39 [-0.37]	-3.47 [1.55]
dimethylsulfoxide	46.826	-6.08	-6.15 [-0.07]	-4.57 [1.51]
n-octanol	9.8629	-5.32	-5.61 [-0.30]	13.74 [19.06]
1,1,1-trichloroethane	7.0826	-4.96	-5.35 [-0.39]	-2.04 [2.92]
1,1,2-trichloroethane	7.1937	-4.98	-5.36 [-0.38]	4.62 [9.60]
1,2,4-trimethylbenzene	2.3653	-2.86	-3.52 [-0.65]	-0.11 [2.75]
1,2-dibromoethane	4.9313	-4.44	-4.94 [-0.49]	4.88 [9.32]
1,2-ethanediol	40.245	-6.04	-6.13 [-0.08]	26.97 [33.02]
1,4-dioxane	2.2099	-2.68	-3.33 [-0.65]	-1.66 [1.01]
1-bromo-2-methylpropane	7.7792	-5.07	-5.43 [-0.36]	-1.82 [3.25]
1-bromooctane	5.0244	-4.48	-4.96 [-0.49]	-0.50 [3.98]
1-bromopentane	6.269	-4.80	-5.22 [-0.42]	-1.11 [3.70]
1-bromopropane	8.0496	-5.11	-5.46 [-0.35]	-1.71 [3.39]
1-butanol	17.332	-5.72	-5.91 [-0.18]	12.66 [18.38]
1-chlorohexane	5.9491	-4.73	-5.17 [-0.44]	-1.07 [3.66]
1-chloropentane	6.5022	-4.85	-5.26 [-0.41]	-1.40 [3.45]
1-chloropropane	8.3548	-5.15	-5.49 [-0.34]	-2.23 [2.92]
1-decanol	7.5305	-5.04	-5.40 [-0.37]	14.48 [19.52]
1-fluorooctane	3.89	-4.02	-4.58 [-0.56]	-0.76 [3.26]
1-heptanol	11.321	-5.43	-5.70 [-0.27]	13.47 [18.90]
1-hexanol	12.51	-5.51	-5.76 [-0.24]	13.17 [18.69]
1-hexene	2.0717	-2.49	-3.14 [-0.65]	-0.20 [2.29]
1-hexyne	2.615	-3.13	-3.77 [-0.65]	5.44 [8.57]
1-iodobutane	6.173	-4.78	-5.21 [-0.43]	-1.04 [3.75]
1-iodohexadecane	3.5338	-3.83	-4.42 [-0.59]	0.46 [4.28]
1-iodopentane	5.6973	-4.67	-5.12 [-0.45]	-0.83 [3.84]
1-iodopropane	6.9626	-4.94	-5.33 [-0.39]	-1.09 [3.85]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-5.87	-6.01 [-0.14]	-2.73 [3.14]
1-nonanol	8.5991	-5.18	-5.51 [-0.33]	14.11 [19.29]
1-pentanol	15.13	-5.64	-5.85 [-0.21]	12.87 [18.51]
1-pentene	1.9905	-2.37	-3.01 [-0.64]	-0.49 [1.88]
1-propanol	20.524	-5.81	-5.97 [-0.16]	12.25 [18.06]
2,2,2-trifluoroethanol	26.726	-5.92	-6.04 [-0.12]	26.53 [32.45]
2,2,4-trimethylpentane	1.9358	-2.29	-2.92 [-0.63]	0.48 [2.77]
2,4-dimethylpentane	1.8939	-2.22	-2.85 [-0.63]	0.43 [2.65]
2,4-dimethylpyridine	9.4176	-5.27	-5.58 [-0.31]	-4.42 [0.85]
2,6-dimethylpyridine	7.1735	-4.98	-5.36 [-0.38]	-4.40 [0.58]
2-bromopropane	9.361	-5.27	-5.58 [-0.31]	-2.31 [2.96]
2-butanol	15.944	-5.68	-5.87 [-0.20]	9.54 [15.22]
2-chlorobutane	8.393	-5.16	-5.50 [-0.34]	-2.28 [2.88]
2-heptanone	11.658	-5.46	-5.72 [-0.26]	-4.28 [1.18]
2-hexanone	14.136	-5.60	-5.82 [-0.22]	-4.52 [1.08]
2-methoxyethanol	17.2	-5.72	-5.90 [-0.18]	7.33 [13.05]
2-methyl-1-propanol	16.777	-5.71	-5.89 [-0.19]	12.30 [18.01]
2-methyl-2-propanol	12.47	-5.51	-5.76 [-0.24]	8.07 [13.58]
2-methylpentane	1.89	-2.22	-2.85 [-0.63]	0.32 [2.53]
2-methylpyridine	9.9533	-5.32	-5.62 [-0.29]	-4.23 [1.09]
2-nitropropane	25.654	-5.90	-6.03 [-0.13]	-3.02 [2.89]
2-octanone	9.4678	-5.28	-5.58 [-0.31]	-4.15 [1.13]
2-pentanone	15.2	-5.65	-5.85 [-0.20]	-4.91 [0.74]
2-propanol	19.264	-5.78	-5.94 [-0.17]	9.11 [14.88]
2-propen-1-ol	19.011	-5.77	-5.94 [-0.17]	13.22 [19.00]
3-methylpyridine	11.645	-5.46	-5.72 [-0.26]	-3.86 [1.59]
3-pentanone	16.78	-5.71	-5.89 [-0.19]	-4.73 [0.98]
4-heptanone	12.257	-5.50	-5.74 [-0.25]	-4.49 [1.00]
4-methyl-2-pentanone	12.887	-5.53	-5.77 [-0.24]	-4.77 [0.77]
4-methylpyridine	11.957	-5.48	-5.73 [-0.25]	-3.82 [1.66]
5-nonanone	10.6	-5.38	-5.66 [-0.28]	-4.19 [1.19]
aceticacid	6.2528	-4.80	-5.22 [-0.42]	29.96 [34.76]
acetophenone	17.44	-5.73	-5.91 [-0.18]	-2.92 [2.80]
2-chlorotoluene	6.7175	-4.90	-5.30 [-0.40]	-1.73 [3.17]
anisole	4.2247	-4.18	-4.72 [-0.54]	-1.07 [3.11]
benzaldehyde	18.22	-5.75	-5.93 [-0.18]	-2.92 [2.83]
benzonitrile	25.592	-5.90	-6.03 [-0.13]	-2.31 [3.59]
benzylalcohol	12.457	-5.51	-5.76 [-0.24]	11.31 [16.82]
bromobenzene	5.3954	-4.59	-5.05 [-0.46]	-0.41 [4.18]
bromoethane	9.01	-5.23	-5.55 [-0.32]	-2.19 [3.04]
bromoform	4.2488	-4.19	-4.73 [-0.54]	8.37 [12.56]
butanal	13.45	-5.57	-5.79 [-0.23]	-4.26 [1.30]
butanoicacid	2.9931	-3.46	-4.08 [-0.62]	31.52 [34.98]
butanone	18.246	-5.75	-5.93 [-0.17]	-4.89 [0.87]
butanonitrile	24.291	-5.88	-6.02 [-0.13]	-3.57 [2.32]
butylamine	4.6178	-4.33	-4.85 [-0.51]	2.92 [7.25]
butylethanoate	4.9941	-4.47	-4.96 [-0.49]	-3.18 [1.28]
carbondisulfide	2.6105	-3.12	-3.77 [-0.65]	1.36 [4.48]
cis-1,2-dimethylcyclohexane	2.06	-2.47	-3.12 [-0.65]	1.42 [3.89]
cis-decalin	2.2139	-2.68	-3.33 [-0.65]	2.26 [4.94]
cyclohexanone	15.619	-5.66	-5.86 [-0.20]	-3.46 [2.21]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-2.33	-2.96 [-0.64]	1.01 [3.34]
cyclopentanol	16.989	-5.71	-5.90 [-0.19]	10.50 [16.22]
cyclopentanone	13.58	-5.57	-5.80 [-0.23]	-3.39 [2.18]
dibromomethane	7.2273	-4.99	-5.37 [-0.38]	4.12 [9.11]
dibutylether	3.0473	-3.50	-4.12 [-0.62]	-2.34 [1.16]
diethylamine	3.5766	-3.85	-4.44 [-0.59]	40.67 [44.52]
diethylsulfide	5.723	-4.68	-5.13 [-0.45]	-2.60 [2.07]
diiodomethane	5.32	-4.57	-5.04 [-0.47]	6.88 [11.45]
diisopropylether	3.38	-3.73	-4.33 [-0.60]	-3.50 [0.23]
dimethyldisulfide	9.6	-5.29	-5.59 [-0.30]	-1.53 [3.76]
diphenylether	3.73	-3.94	-4.51 [-0.57]	-2.05 [1.89]
dipropylamine	2.9112	-3.39	-4.02 [-0.63]	-0.33 [3.07]
E-1,2-dichloroethene	2.14	-2.58	-3.23 [-0.65]	5.27 [7.86]
E-2-pentene	2.051	-2.46	-3.11 [-0.65]	-0.41 [2.05]
ethanethiol	6.667	-4.89	-5.29 [-0.40]	-2.51 [2.38]
ethylbenzene	2.4339	-2.94	-3.59 [-0.65]	-0.14 [2.80]
ethylethanoate	5.9867	-4.74	-5.17 [-0.43]	-3.65 [1.09]
ethylmethanoate	8.331	-5.15	-5.49 [-0.34]	-3.60 [1.55]
ethylphenylether	4.1797	-4.16	-4.70 [-0.54]	-1.52 [2.64]
fluorobenzene	5.42	-4.59	-5.06 [-0.46]	-1.81 [2.78]
formamide	108.94	-6.20	-6.24 [-0.03]	31.78 [37.99]
formicacid	51.1	-6.10	-6.16 [-0.07]	38.30 [44.40]
hexanoicacid	2.6	-3.11	-3.76 [-0.65]	32.37 [35.48]
iodobenzene	4.547	-4.31	-4.83 [-0.52]	0.21 [4.52]
iodoethane	7.6177	-5.05	-5.41 [-0.36]	-1.25 [3.80]
iodomethane	6.865	-4.92	-5.32 [-0.39]	-0.72 [4.21]
isopropylbenzene	2.3712	-2.87	-3.52 [-0.65]	-0.16 [2.71]
m-cresol	12.44	-5.51	-5.75 [-0.24]	27.38 [32.89]
mesitylene	2.265	-2.74	-3.40 [-0.65]	-0.28 [2.46]
methylbenzoate	6.7367	-4.90	-5.30 [-0.40]	-2.20 [2.70]
methylbutanoate	5.5607	-4.63	-5.09 [-0.46]	-3.37 [1.27]
methylcyclohexane	2.024	-2.42	-3.06 [-0.64]	1.16 [3.58]
methylethanoate	6.8615	-4.92	-5.32 [-0.39]	-3.60 [1.33]
methylmethanoate	8.8377	-5.21	-5.53 [-0.33]	-3.45 [1.76]
methylpropanoate	6.0777	-4.76	-5.19 [-0.43]	-3.51 [1.25]
m-xylene	2.3478	-2.84	-3.49 [-0.65]	-0.17 [2.67]
n-butylbenzene	2.36	-2.86	-3.51 [-0.65]	0.19 [3.05]
n-decane	1.9846	-2.36	-3.00 [-0.64]	1.22 [3.59]
n-dodecane	2.006	-2.39	-3.04 [-0.64]	1.44 [3.84]
n-hexadecane	2.0402	-2.44	-3.09 [-0.65]	1.74 [4.18]
n-hexane	1.8819	-2.20	-2.83 [-0.63]	0.49 [2.69]
nitrobenzene	34.809	-6.01	-6.10 [-0.09]	-1.75 [4.25]
nitroethane	28.29	-5.94	-6.06 [-0.12]	-1.80 [4.14]
N-methylaniline	5.96	-4.73	-5.17 [-0.44]	5.27 [10.01]
N,N-dimethylacetamide	37.781	-6.03	-6.12 [-0.09]	-5.47 [0.56]
N,N-dimethylformamide	37.219	-6.03	-6.11 [-0.09]	-4.98 [1.04]
n-nonane	1.9605	-2.33	-2.96 [-0.64]	1.09 [3.42]
n-octane	1.9406	-2.30	-2.93 [-0.63]	0.92 [3.22]
n-pentadecane	2.0333	-2.44	-3.08 [-0.64]	1.68 [4.12]
n-pentane	1.8371	-2.13	-2.75 [-0.62]	0.17 [2.30]
n-undecane	1.991	-2.37	-3.01 [-0.64]	1.34 [3.71]

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solvent	$\varepsilon/\varepsilon_o$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-4.34	-4.85 [-0.51]	-0.17 [4.17]
o-cresol	6.76	-4.90	-5.30 [-0.40]	25.83 [30.74]
o-dichlorobenzene	9.9949	-5.33	-5.62 [-0.29]	-0.38 [4.94]
o-nitrotoluene	25.669	-5.90	-6.03 [-0.13]	-1.29 [4.61]
o-xylene	2.5454	-3.06	-3.71 [-0.65]	-0.14 [2.91]
pentanal	10	-5.33	-5.62 [-0.29]	-3.87 [1.46]
pentanoicacid	2.6924	-3.20	-3.84 [-0.64]	32.08 [35.28]
pentylamine	4.201	-4.17	-4.71 [-0.54]	3.35 [7.52]
pentylethanoate	4.7297	-4.38	-4.88 [-0.51]	-3.06 [1.32]
perfluorobenzene	2.029	-2.43	-3.07 [-0.64]	0.11 [2.54]
p-isopropyltoluene	2.2322	-2.70	-3.36 [-0.65]	-0.28 [2.43]
propanal	18.5	-5.76	-5.93 [-0.17]	-4.72 [1.04]
propanoicacid	3.44	-3.77	-4.36 [-0.60]	30.99 [34.76]
propanonitrile	29.324	-5.95	-6.06 [-0.11]	-2.86 [3.09]
propylamine	4.9912	-4.47	-4.96 [-0.49]	2.46 [6.93]
propylethanoate	5.5205	-4.62	-5.08 [-0.46]	-3.49 [1.13]
p-xylene	2.2705	-2.75	-3.40 [-0.65]	-0.17 [2.58]
pyridine	12.978	-5.54	-5.78 [-0.24]	-3.73 [1.81]
sec-butylbenzene	2.3446	-2.84	-3.49 [-0.65]	0.03 [2.87]
tert-butylbenzene	2.3447	-2.84	-3.49 [-0.65]	-0.03 [2.81]
tetrachloroethene	2.268	-2.75	-3.40 [-0.65]	1.21 [3.96]
tetrahydrothiophene-S,S-dioxide	43.962	-6.06	-6.14 [-0.08]	-1.71 [4.36]
tetralin	2.771	-3.27	-3.91 [-0.64]	0.29 [3.56]
thiophene	2.727	-3.23	-3.88 [-0.64]	-0.19 [3.04]
thiophenol	4.2728	-4.20	-4.73 [-0.54]	4.13 [8.33]
trans-decalin	2.1781	-2.63	-3.28 [-0.65]	1.94 [4.57]
tributylphosphate	8.1781	-5.13	-5.47 [-0.35]	-9.65 [-4.52]
trichloroethene	3.422	-3.76	-4.36 [-0.60]	3.76 [7.52]
triethylamine	2.3832	-2.88	-3.54 [-0.65]	-4.81 [-1.93]
xylenemixture	2.3879	-2.89	-3.54 [-0.65]	-0.17 [2.72]
Z-1,2-dichloroethene	9.2	-5.25	-5.56 [-0.32]	3.15 [8.40]

Table 3. Calculated standard state (298.15 K, 1 mol L^{-1} → 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for sulfur dioxide (SO_2) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_o$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-13.11	-13.32 [-0.20]	-14.44 [-1.32]
methanol	32.613	-13.05	-13.27 [-0.22]	-3.48 [9.57]
ethanol	24.852	-12.84	-13.12 [-0.28]	-6.29 [6.54]
isoquinoline	11	-11.74	-12.31 [-0.57]	-15.28 [-3.54]
quinoline	9.16	-11.36	-12.02 [-0.66]	-15.06 [-3.70]
chloroform	4.7113	-9.39	-10.44 [-1.05]	-8.69 [0.70]
diethylether	4.24	-8.97	-10.08 [-1.11]	-17.61 [-8.63]
dichloromethane	8.93	-11.30	-11.98 [-0.68]	-11.53 [-0.23]
dichloroethane	10.125	-11.57	-12.19 [-0.61]	-11.17 [0.40]
carbontetrachloride	2.228	-5.72	-7.01 [-1.29]	-12.28 [-6.56]
benzene	2.2706	-5.83	-7.13 [-1.30]	-13.72 [-7.89]
toluene	2.3741	-6.10	-7.40 [-1.30]	-13.49 [-7.39]
chlorobenzene	5.6968	-10.06	-11.00 [-0.94]	-14.52 [-4.46]
nitromethane	36.562	-13.13	-13.33 [-0.20]	-13.60 [-0.47]
heptane	1.9113	-4.75	-5.99 [-1.24]	-10.80 [-6.05]
cyclohexane	2.0165	-5.10	-6.36 [-1.26]	-10.43 [-5.33]
aniline	6.8882	-10.64	-11.46 [-0.82]	-7.49 [3.15]
acetone	20.493	-12.64	-12.98 [-0.34]	-17.96 [-5.31]
tetrahydrofuran	7.4257	-10.85	-11.63 [-0.78]	-17.91 [-7.06]
dimethylsulfoxide	46.826	-13.27	-13.42 [-0.15]	-20.59 [-7.33]
n-octanol	9.8629	-11.52	-12.15 [-0.63]	-4.87 [6.65]
1,1,1-trichloroethane	7.0826	-10.72	-11.52 [-0.81]	-15.50 [-4.78]
1,1,2-trichloroethane	7.1937	-10.76	-11.56 [-0.80]	-9.85 [0.91]
1,2,4-trimethylbenzene	2.3653	-6.08	-7.38 [-1.30]	-13.39 [-7.31]
1,2-dibromoethane	4.9313	-9.56	-10.58 [-1.02]	-9.87 [-0.31]
1,2-ethanediol	40.245	-13.19	-13.37 [-0.18]	3.67 [16.86]
1,4-dioxane	2.2099	-5.67	-6.96 [-1.29]	-15.62 [-9.95]
1-bromo-2-methylpropane	7.7792	-10.97	-11.72 [-0.75]	-15.35 [-4.38]
1-bromooctane	5.0244	-9.63	-10.64 [-1.01]	-13.82 [-4.20]
1-bromopentane	6.269	-10.36	-11.24 [-0.88]	-14.55 [-4.19]
1-bromopropane	8.0496	-11.05	-11.79 [-0.73]	-15.24 [-4.19]
1-butanol	17.332	-12.45	-12.84 [-0.39]	-5.76 [6.68]
1-chlorohexane	5.9491	-10.20	-11.11 [-0.91]	-14.24 [-4.04]
1-chloropentane	6.5022	-10.47	-11.33 [-0.86]	-14.60 [-4.12]
1-chloropropane	8.3548	-11.14	-11.86 [-0.71]	-15.42 [-4.28]
1-decanol	7.5305	-10.88	-11.65 [-0.77]	-4.16 [6.72]
1-fluorooctane	3.89	-8.61	-9.77 [-1.16]	-13.46 [-4.84]
1-heptanol	11.321	-11.79	-12.35 [-0.56]	-5.11 [6.68]
1-hexanol	12.51	-11.97	-12.48 [-0.52]	-5.37 [6.60]
1-hexene	2.0717	-5.27	-6.55 [-1.27]	-12.08 [-6.81]
1-hexyne	2.615	-6.65	-7.94 [-1.29]	-8.25 [-1.60]
1-iodobutane	6.173	-10.32	-11.20 [-0.89]	-14.97 [-4.65]
1-iodohexadecane	3.5338	-8.18	-9.38 [-1.20]	-12.83 [-4.64]
1-iodopentane	5.6973	-10.06	-11.00 [-0.94]	-14.67 [-4.61]
1-iodopropane	6.9626	-10.67	-11.49 [-0.82]	-15.12 [-4.45]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-12.79	-13.09 [-0.29]	-16.85 [-4.06]
1-nonanol	8.5991	-11.21	-11.91 [-0.70]	-4.51 [6.71]
1-pentanol	15.13	-12.26	-12.70 [-0.44]	-5.63 [6.64]
1-pentene	1.9905	-5.02	-6.27 [-1.26]	-12.27 [-7.25]
1-propanol	20.524	-12.65	-12.98 [-0.33]	-6.09 [6.55]
2,2,2-trifluoroethanol	26.726	-12.90	-13.16 [-0.26]	5.92 [18.82]
2,2,4-trimethylpentane	1.9358	-4.84	-6.08 [-1.24]	-11.12 [-6.28]
2,4-dimethylpentane	1.8939	-4.69	-5.93 [-1.23]	-11.07 [-6.38]
2,4-dimethylpyridine	9.4176	-11.42	-12.07 [-0.65]	-20.18 [-8.76]
2,6-dimethylpyridine	7.1735	-10.75	-11.55 [-0.80]	-20.02 [-9.27]
2-bromopropane	9.361	-11.41	-12.06 [-0.65]	-15.93 [-4.52]
2-butanol	15.944	-12.34	-12.76 [-0.42]	-8.47 [3.86]
2-chlorobutane	8.393	-11.16	-11.87 [-0.71]	-15.60 [-4.44]
2-heptanone	11.658	-11.84	-12.39 [-0.55]	-19.05 [-7.20]
2-hexanone	14.136	-12.16	-12.63 [-0.46]	-19.29 [-7.13]
2-methoxyethanol	17.2	-12.44	-12.83 [-0.39]	-11.01 [1.43]
2-methyl-1-propanol	16.777	-12.41	-12.81 [-0.40]	-6.13 [6.27]
2-methyl-2-propanol	12.47	-11.96	-12.48 [-0.52]	-9.71 [2.25]
2-methylpentane	1.89	-4.68	-5.91 [-1.23]	-11.12 [-6.44]
2-methylpyridine	9.9533	-11.54	-12.16 [-0.62]	-19.81 [-8.27]
2-nitropropane	25.654	-12.87	-13.14 [-0.27]	-17.18 [-4.31]
2-octanone	9.4678	-11.43	-12.08 [-0.65]	-18.90 [-7.47]
2-pentanone	15.2	-12.27	-12.71 [-0.44]	-19.65 [-7.38]
2-propanol	19.264	-12.58	-12.93 [-0.35]	-8.78 [3.80]
2-propen-1-ol	19.011	-12.56	-12.92 [-0.36]	-5.50 [7.06]
3-methylpyridine	11.645	-11.84	-12.39 [-0.55]	-19.39 [-7.55]
3-pentanone	16.78	-12.41	-12.81 [-0.40]	-19.49 [-7.08]
4-heptanone	12.257	-11.93	-12.46 [-0.53]	-19.28 [-7.35]
4-methyl-2-pentanone	12.887	-12.02	-12.52 [-0.50]	-19.51 [-7.50]
4-methylpyridine	11.957	-11.89	-12.42 [-0.54]	-19.35 [-7.46]
5-nonanone	10.6	-11.66	-12.26 [-0.59]	-19.00 [-7.34]
aceticacid	6.2528	-10.36	-11.23 [-0.88]	7.45 [17.80]
acetophenone	17.44	-12.46	-12.84 [-0.39]	-18.52 [-6.06]
2-chlorotoluene	6.7175	-10.57	-11.41 [-0.84]	-16.55 [-5.98]
anisole	4.2247	-8.96	-10.07 [-1.11]	-15.31 [-6.35]
benzaldehyde	18.22	-12.51	-12.88 [-0.37]	-18.35 [-5.84]
benzonitrile	25.592	-12.86	-13.14 [-0.28]	-17.42 [-4.56]
benzylalcohol	12.457	-11.96	-12.48 [-0.52]	-7.63 [4.33]
bromobenzene	5.3954	-9.88	-10.85 [-0.97]	-14.50 [-4.62]
bromoethane	9.01	-11.32	-11.99 [-0.67]	-15.72 [-4.40]
bromoform	4.2488	-8.98	-10.09 [-1.11]	-6.83 [2.15]
butanal	13.45	-12.09	-12.57 [-0.49]	-18.71 [-6.62]
butanoicacid	2.9931	-7.37	-8.64 [-1.27]	8.95 [16.32]
butanone	18.246	-12.51	-12.88 [-0.37]	-19.58 [-7.06]
butanonitrile	24.291	-12.82	-13.10 [-0.29]	-17.79 [-4.97]
butylamine	4.6178	-9.31	-10.37 [-1.06]	-12.99 [-3.68]
butylethanoate	4.9941	-9.60	-10.62 [-1.01]	-17.24 [-7.64]
carbondisulfide	2.6105	-6.64	-7.94 [-1.30]	-12.50 [-5.86]
cis-1,2-dimethylcyclohexane	2.06	-5.24	-6.51 [-1.27]	-10.49 [-5.26]
cis-decalin	2.2139	-5.68	-6.97 [-1.29]	-9.99 [-4.31]
cyclohexanone	15.619	-12.31	-12.74 [-0.43]	-18.65 [-6.34]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-4.92	-6.17 [-1.25]	-10.66 [-5.74]
cyclopentanol	16.989	-12.42	-12.82 [-0.40]	-7.59 [4.83]
cyclopentanone	13.58	-12.10	-12.58 [-0.48]	-18.33 [-6.23]
dibromomethane	7.2273	-10.77	-11.57 [-0.80]	-10.54 [0.24]
dibutylether	3.0473	-7.46	-8.72 [-1.26]	-16.00 [-8.54]
diethylamine	3.5766	-8.24	-9.43 [-1.20]	13.58 [21.82]
diethylsulfide	5.723	-10.07	-11.01 [-0.93]	-16.69 [-6.62]
diiodomethane	5.32	-9.83	-10.80 [-0.97]	-8.82 [1.01]
diisopropylether	3.38	-7.97	-9.19 [-1.22]	-17.03 [-9.06]
dimethyldisulfide	9.6	-11.46	-12.10 [-0.64]	-16.24 [-4.78]
diphenylether	3.73	-8.43	-9.60 [-1.17]	-16.54 [-8.11]
dipropylamine	2.9112	-7.23	-8.50 [-1.27]	-15.66 [-8.43]
E-1,2-dichloroethene	2.14	-5.47	-6.76 [-1.28]	-8.10 [-2.63]
E-2-pentene	2.051	-5.21	-6.48 [-1.27]	-12.27 [-7.07]
ethanethiol	6.667	-10.54	-11.39 [-0.84]	-16.35 [-5.80]
ethylbenzene	2.4339	-6.24	-7.54 [-1.30]	-13.27 [-7.03]
ethylethanoate	5.9867	-10.22	-11.12 [-0.91]	-17.69 [-7.47]
ethylmethanoate	8.331	-11.14	-11.85 [-0.71]	-17.47 [-6.34]
ethylphenylether	4.1797	-8.92	-10.03 [-1.12]	-15.80 [-6.89]
fluorobenzene	5.42	-9.89	-10.86 [-0.96]	-15.39 [-5.50]
formamide	108.94	-13.55	-13.62 [-0.07]	8.38 [21.93]
formicacid	51.1	-13.31	-13.45 [-0.14]	13.48 [26.79]
hexanoicacid	2.6	-6.62	-7.91 [-1.30]	9.68 [16.30]
iodobenzene	4.547	-9.25	-10.32 [-1.07]	-14.26 [-5.00]
iodoethane	7.6177	-10.91	-11.68 [-0.77]	-15.39 [-4.48]
iodomethane	6.865	-10.63	-11.46 [-0.83]	-14.89 [-4.26]
isopropylbenzene	2.3712	-6.09	-7.39 [-1.30]	-13.26 [-7.17]
m-cresol	12.44	-11.96	-12.48 [-0.52]	4.64 [16.60]
mesitylene	2.265	-5.82	-7.12 [-1.30]	-13.49 [-7.67]
methylbenzoate	6.7367	-10.58	-11.41 [-0.83]	-17.26 [-6.68]
methylbutanoate	5.5607	-9.98	-10.93 [-0.95]	-17.46 [-7.48]
methylcyclohexane	2.024	-5.13	-6.39 [-1.26]	-10.66 [-5.54]
methylethanoate	6.8615	-10.63	-11.45 [-0.82]	-17.60 [-6.97]
methylmethanoate	8.8377	-11.28	-11.96 [-0.68]	-17.20 [-5.93]
methylpropanoate	6.0777	-10.27	-11.16 [-0.90]	-17.57 [-7.31]
m-xylene	2.3478	-6.03	-7.33 [-1.30]	-13.31 [-7.28]
n-butylbenzene	2.36	-6.06	-7.36 [-1.30]	-12.82 [-6.76]
n-decane	1.9846	-5.00	-6.25 [-1.25]	-10.47 [-5.47]
n-dodecane	2.006	-5.07	-6.33 [-1.26]	-10.33 [-5.26]
n-hexadecane	2.0402	-5.17	-6.44 [-1.27]	-10.11 [-4.94]
n-hexane	1.8819	-4.66	-5.88 [-1.23]	-10.95 [-6.30]
nitrobenzene	34.809	-13.10	-13.30 [-0.20]	-16.90 [-3.80]
nitroethane	28.29	-12.95	-13.20 [-0.25]	-15.98 [-3.04]
N-methylaniline	5.96	-10.21	-11.11 [-0.91]	-11.24 [-1.04]
N,N-dimethylacetamide	37.781	-13.15	-13.34 [-0.19]	-21.47 [-8.32]
N,N-dimethylformamide	37.219	-13.14	-13.33 [-0.19]	-20.77 [-7.63]
n-nonane	1.9605	-4.92	-6.17 [-1.25]	-10.56 [-5.64]
n-octane	1.9406	-4.85	-6.10 [-1.24]	-10.68 [-5.82]
n-pentadecane	2.0333	-5.15	-6.42 [-1.27]	-10.15 [-5.00]
n-pentane	1.8371	-4.49	-5.71 [-1.21]	-11.14 [-6.65]
n-undecane	1.991	-5.02	-6.28 [-1.26]	-10.57 [-5.55]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-9.33	-10.38 [-1.06]	-13.85 [-4.52]
o-cresol	6.76	-10.59	-11.42 [-0.83]	4.28 [14.86]
o-dichlorobenzene	9.9949	-11.54	-12.17 [-0.62]	-14.51 [-2.96]
o-nitrotoluene	25.669	-12.87	-13.14 [-0.27]	-16.25 [-3.39]
o-xylene	2.5454	-6.50	-7.80 [-1.30]	-13.42 [-6.93]
pentanal	10	-11.55	-12.17 [-0.62]	-18.28 [-6.74]
pentanoicacid	2.6924	-6.81	-8.10 [-1.29]	9.43 [16.24]
pentylamine	4.201	-8.94	-10.05 [-1.11]	-12.88 [-3.94]
pentylethanoate	4.7297	-9.40	-10.45 [-1.04]	-17.14 [-7.74]
perfluorobenzene	2.029	-5.14	-6.41 [-1.27]	-11.48 [-6.34]
p-isopropyltoluene	2.2322	-5.73	-7.02 [-1.29]	-13.40 [-7.67]
propanal	18.5	-12.53	-12.90 [-0.37]	-19.12 [-6.59]
propanoicacid	3.44	-8.06	-9.27 [-1.22]	8.51 [16.57]
propanonitrile	29.324	-12.98	-13.22 [-0.24]	-17.04 [-4.07]
propylamine	4.9912	-9.60	-10.62 [-1.02]	-13.36 [-3.75]
propylethanoate	5.5205	-9.96	-10.91 [-0.95]	-17.56 [-7.60]
p-xylene	2.2705	-5.83	-7.13 [-1.29]	-13.26 [-7.43]
pyridine	12.978	-12.03	-12.53 [-0.50]	-19.25 [-7.23]
sec-butylbenzene	2.3446	-6.03	-7.32 [-1.30]	-13.02 [-6.99]
tert-butylbenzene	2.3447	-6.03	-7.33 [-1.30]	-13.11 [-7.09]
tetrachloroethene	2.268	-5.83	-7.12 [-1.30]	-11.37 [-5.54]
tetrahydrothiophene-S,S-dioxide	43.962	-13.24	-13.40 [-0.17]	-17.93 [-4.69]
tetralin	2.771	-6.97	-8.25 [-1.29]	-13.38 [-6.42]
thiophene	2.727	-6.88	-8.17 [-1.29]	-13.69 [-6.82]
thiophenol	4.2728	-9.01	-10.11 [-1.10]	-10.91 [-1.91]
trans-decalin	2.1781	-5.58	-6.87 [-1.29]	-10.24 [-4.66]
tributylphosphate	8.1781	-11.09	-11.82 [-0.72]	-26.90 [-15.80]
trichloroethene	3.422	-8.03	-9.25 [-1.22]	-9.93 [-1.90]
triethylamine	2.3832	-6.12	-7.42 [-1.30]	-19.44 [-13.32]
xylenemixture	2.3879	-6.13	-7.43 [-1.30]	-13.34 [-7.21]
Z-1,2-dichloroethene	9.2	-11.37	-12.03 [-0.66]	-10.87 [0.49]

Table 4. Calculated standard state (298.15 K, 1 mol L^{-1} → 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for dioxygen (O_2) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-0.22	-0.22 [0.00]	-10.02 [-9.80]
methanol	32.613	-0.22	-0.22 [-0.01]	0.48 [0.70]
ethanol	24.852	-0.22	-0.22 [-0.01]	-2.37 [-2.15]
isoquinoline	11	-0.20	-0.21 [-0.01]	-4.56 [-4.36]
quinoline	9.16	-0.19	-0.20 [-0.02]	-4.56 [-4.37]
chloroform	4.7113	-0.15	-0.18 [-0.03]	2.58 [2.74]
diethylether	4.24	-0.15	-0.18 [-0.03]	-18.10 [-17.95]
dichloromethane	8.93	-0.19	-0.20 [-0.02]	-0.54 [-0.35]
dichloroethane	10.125	-0.19	-0.21 [-0.01]	-1.77 [-1.58]
carbontetrachloride	2.228	-0.09	-0.13 [-0.03]	-4.26 [-4.17]
benzene	2.2706	-0.10	-0.13 [-0.03]	-9.02 [-8.92]
toluene	2.3741	-0.10	-0.13 [-0.03]	-8.75 [-8.65]
chlorobenzene	5.6968	-0.17	-0.19 [-0.02]	-5.87 [-5.70]
nitromethane	36.562	-0.22	-0.23 [-0.01]	-9.32 [-9.09]
heptane	1.9113	-0.08	-0.11 [-0.03]	-3.71 [-3.63]
cyclohexane	2.0165	-0.08	-0.12 [-0.03]	-3.25 [-3.16]
aniline	6.8882	-0.18	-0.20 [-0.02]	-4.07 [-3.90]
acetone	20.493	-0.21	-0.22 [-0.01]	-18.07 [-17.86]
tetrahydrofuran	7.4257	-0.18	-0.20 [-0.02]	-19.37 [-19.19]
dimethylsulfoxide	46.826	-0.22	-0.23 [0.00]	-31.23 [-31.01]
n-octanol	9.8629	-0.19	-0.21 [-0.02]	-1.93 [-1.74]
1,1,1-trichloroethane	7.0826	-0.18	-0.20 [-0.02]	-6.97 [-6.79]
1,1,2-trichloroethane	7.1937	-0.18	-0.20 [-0.02]	-1.02 [-0.85]
1,2,4-trimethylbenzene	2.3653	-0.10	-0.13 [-0.03]	-10.04 [-9.94]
1,2-dibromoethane	4.9313	-0.16	-0.18 [-0.03]	-3.25 [-3.10]
1,2-ethanediol	40.245	-0.22	-0.23 [-0.01]	0.02 [0.24]
1,4-dioxane	2.2099	-0.09	-0.13 [-0.03]	-24.25 [-24.16]
1-bromo-2-methylpropane	7.7792	-0.18	-0.20 [-0.02]	-7.59 [-7.40]
1-bromooctane	5.0244	-0.16	-0.18 [-0.02]	-7.02 [-6.86]
1-bromopentane	6.269	-0.17	-0.19 [-0.02]	-7.25 [-7.08]
1-bromopropane	8.0496	-0.18	-0.20 [-0.02]	-7.47 [-7.29]
1-butanol	17.332	-0.21	-0.22 [-0.01]	-2.13 [-1.92]
1-chlorohexane	5.9491	-0.17	-0.19 [-0.02]	-6.58 [-6.41]
1-chloropentane	6.5022	-0.17	-0.19 [-0.02]	-6.74 [-6.56]
1-chloropropane	8.3548	-0.19	-0.20 [-0.02]	-7.09 [-6.90]
1-decanol	7.5305	-0.18	-0.20 [-0.02]	-1.75 [-1.57]
1-fluorooctane	3.89	-0.14	-0.17 [-0.03]	-6.72 [-6.58]
1-heptanol	11.321	-0.20	-0.21 [-0.01]	-1.97 [-1.78]
1-hexanol	12.51	-0.20	-0.21 [-0.01]	-2.07 [-1.87]
1-hexene	2.0717	-0.09	-0.12 [-0.03]	-6.34 [-6.25]
1-hexyne	2.615	-0.11	-0.14 [-0.03]	-1.30 [-1.19]
1-iodobutane	6.173	-0.17	-0.19 [-0.02]	-8.31 [-8.14]
1-iodohexadecane	3.5338	-0.14	-0.17 [-0.03]	-7.69 [-7.56]
1-iodopentane	5.6973	-0.17	-0.19 [-0.02]	-8.21 [-8.04]
1-iodopropane	6.9626	-0.18	-0.20 [-0.02]	-8.27 [-8.09]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-0.22	-0.22 [-0.01]	-13.16 [-12.94]
1-nonanol	8.5991	-0.19	-0.20 [-0.02]	-1.83 [-1.64]
1-pentanol	15.13	-0.20	-0.22 [-0.01]	-2.11 [-1.91]
1-pentene	1.9905	-0.08	-0.11 [-0.03]	-6.59 [-6.51]
1-propanol	20.524	-0.21	-0.22 [-0.01]	-2.29 [-2.07]
2,2,2-trifluoroethanol	26.726	-0.22	-0.22 [-0.01]	15.62 [15.84]
2,2,4-trimethylpentane	1.9358	-0.08	-0.11 [-0.03]	-3.90 [-3.82]
2,4-dimethylpentane	1.8939	-0.08	-0.11 [-0.03]	-3.94 [-3.86]
2,4-dimethylpyridine	9.4176	-0.19	-0.20 [-0.01]	-24.73 [-24.54]
2,6-dimethylpyridine	7.1735	-0.18	-0.20 [-0.02]	-24.90 [-24.72]
2-bromopropane	9.361	-0.19	-0.20 [-0.02]	-8.38 [-8.19]
2-butanol	15.944	-0.21	-0.22 [-0.01]	-6.94 [-6.73]
2-chlorobutane	8.393	-0.19	-0.20 [-0.02]	-7.74 [-7.55]
2-heptanone	11.658	-0.20	-0.21 [-0.01]	-20.59 [-20.39]
2-hexanone	14.136	-0.20	-0.22 [-0.01]	-20.64 [-20.44]
2-methoxyethanol	17.2	-0.21	-0.22 [-0.01]	-16.91 [-16.71]
2-methyl-1-propanol	16.777	-0.21	-0.22 [-0.01]	-2.43 [-2.22]
2-methyl-2-propanol	12.47	-0.20	-0.21 [-0.01]	-9.50 [-9.30]
2-methylpentane	1.89	-0.08	-0.11 [-0.03]	-3.99 [-3.92]
2-methylpyridine	9.9533	-0.19	-0.21 [-0.02]	-23.05 [-22.86]
2-nitropropane	25.654	-0.22	-0.22 [-0.01]	-13.92 [-13.71]
2-octanone	9.4678	-0.19	-0.21 [-0.02]	-20.64 [-20.45]
2-pentanone	15.2	-0.20	-0.22 [-0.01]	-20.88 [-20.67]
2-propanol	19.264	-0.21	-0.22 [-0.01]	-7.07 [-6.86]
2-propen-1-ol	19.011	-0.21	-0.22 [-0.01]	-1.73 [-1.52]
3-methylpyridine	11.645	-0.20	-0.21 [-0.01]	-21.52 [-21.33]
3-pentanone	16.78	-0.21	-0.22 [-0.01]	-20.70 [-20.49]
4-heptanone	12.257	-0.20	-0.21 [-0.01]	-20.73 [-20.53]
4-methyl-2-pentanone	12.887	-0.20	-0.21 [-0.01]	-20.87 [-20.67]
4-methylpyridine	11.957	-0.20	-0.21 [-0.01]	-21.47 [-21.27]
5-nonanone	10.6	-0.19	-0.21 [-0.02]	-20.62 [-20.42]
aceticacid	6.2528	-0.17	-0.19 [-0.02]	11.09 [11.26]
acetophenone	17.44	-0.21	-0.22 [-0.01]	-18.95 [-18.74]
2-chlorotoluene	6.7175	-0.18	-0.20 [-0.02]	-14.21 [-14.04]
anisole	4.2247	-0.15	-0.18 [-0.03]	-12.93 [-12.78]
benzaldehyde	18.22	-0.21	-0.22 [-0.01]	-16.33 [-16.12]
benzonitrile	25.592	-0.22	-0.22 [-0.01]	-13.90 [-13.69]
benzylalcohol	12.457	-0.20	-0.21 [-0.01]	-6.33 [-6.13]
bromobenzene	5.3954	-0.17	-0.19 [-0.02]	-6.43 [-6.26]
bromoethane	9.01	-0.19	-0.20 [-0.02]	-7.72 [-7.53]
bromoform	4.2488	-0.15	-0.18 [-0.03]	2.85 [3.00]
butanal	13.45	-0.20	-0.21 [-0.01]	-18.64 [-18.44]
butanoicacid	2.9931	-0.12	-0.15 [-0.03]	10.30 [10.42]
butanone	18.246	-0.21	-0.22 [-0.01]	-20.74 [-20.53]
butanonitrile	24.291	-0.22	-0.22 [-0.01]	-15.21 [-15.00]
butylamine	4.6178	-0.15	-0.18 [-0.03]	-16.54 [-16.38]
butylethanoate	4.9941	-0.16	-0.18 [-0.02]	-18.60 [-18.44]
carbondisulfide	2.6105	-0.11	-0.14 [-0.03]	-5.69 [-5.58]
cis-1,2-dimethylcyclohexane	2.06	-0.09	-0.12 [-0.03]	-3.22 [-3.13]
cis-decalin	2.2139	-0.09	-0.13 [-0.03]	-2.60 [-2.51]
cyclohexanone	15.619	-0.20	-0.22 [-0.01]	-21.42 [-21.21]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-0.08	-0.11 [-0.03]	-3.51 [-3.43]
cyclopentanol	16.989	-0.21	-0.22 [-0.01]	-6.36 [-6.15]
cyclopentanone	13.58	-0.20	-0.21 [-0.01]	-20.20 [-20.00]
dibromomethane	7.2273	-0.18	-0.20 [-0.02]	-1.26 [-1.08]
dibutylether	3.0473	-0.12	-0.15 [-0.03]	-18.60 [-18.48]
diethylamine	3.5766	-0.14	-0.17 [-0.03]	11.04 [11.17]
diethylsulfide	5.723	-0.17	-0.19 [-0.02]	-14.39 [-14.22]
diiodomethane	5.32	-0.16	-0.19 [-0.02]	-4.83 [-4.67]
diisopropylether	3.38	-0.13	-0.16 [-0.03]	-18.08 [-17.95]
dimethyldisulfide	9.6	-0.19	-0.21 [-0.02]	-12.26 [-12.07]
diphenylether	3.73	-0.14	-0.17 [-0.03]	-11.48 [-11.34]
dipropylamine	2.9112	-0.12	-0.15 [-0.03]	-23.33 [-23.21]
E-1,2-dichloroethene	2.14	-0.09	-0.12 [-0.03]	-0.92 [-0.83]
E-2-pentene	2.051	-0.09	-0.12 [-0.03]	-6.51 [-6.42]
ethanethiol	6.667	-0.18	-0.20 [-0.02]	-11.77 [-11.59]
ethylbenzene	2.4339	-0.10	-0.13 [-0.03]	-8.81 [-8.70]
ethylethanoate	5.9867	-0.17	-0.19 [-0.02]	-18.70 [-18.53]
ethylmethanoate	8.331	-0.19	-0.20 [-0.02]	-16.27 [-16.08]
ethylphenylether	4.1797	-0.15	-0.18 [-0.03]	-14.14 [-13.99]
fluorobenzene	5.42	-0.17	-0.19 [-0.02]	-7.46 [-7.30]
formamide	108.94	-0.23	-0.23 [0.00]	9.25 [9.48]
formicacid	51.1	-0.22	-0.23 [0.00]	21.04 [21.27]
hexanoicacid	2.6	-0.11	-0.14 [-0.03]	10.49 [10.60]
iodobenzene	4.547	-0.15	-0.18 [-0.03]	-7.25 [-7.09]
iodoethane	7.6177	-0.18	-0.20 [-0.02]	-8.34 [-8.16]
iodomethane	6.865	-0.18	-0.20 [-0.02]	-7.52 [-7.35]
isopropylbenzene	2.3712	-0.10	-0.13 [-0.03]	-9.14 [-9.04]
m-cresol	12.44	-0.20	-0.21 [-0.01]	12.14 [12.34]
mesitylene	2.265	-0.09	-0.13 [-0.03]	-10.23 [-10.13]
methylbenzoate	6.7367	-0.18	-0.20 [-0.02]	-18.31 [-18.13]
methylbutanoate	5.5607	-0.17	-0.19 [-0.02]	-18.61 [-18.45]
methylcyclohexane	2.024	-0.08	-0.12 [-0.03]	-3.41 [-3.32]
methylethanoate	6.8615	-0.18	-0.20 [-0.02]	-18.48 [-18.31]
methylmethanoate	8.8377	-0.19	-0.20 [-0.02]	-16.04 [-15.85]
methylpropanoate	6.0777	-0.17	-0.19 [-0.02]	-18.59 [-18.42]
m-xylene	2.3478	-0.10	-0.13 [-0.03]	-9.19 [-9.09]
n-butylbenzene	2.36	-0.10	-0.13 [-0.03]	-8.57 [-8.47]
n-decane	1.9846	-0.08	-0.11 [-0.03]	-3.34 [-3.26]
n-dodecane	2.006	-0.08	-0.12 [-0.03]	-3.19 [-3.11]
n-hexadecane	2.0402	-0.08	-0.12 [-0.03]	-2.97 [-2.89]
n-hexane	1.8819	-0.08	-0.11 [-0.03]	-3.88 [-3.80]
nitrobenzene	34.809	-0.22	-0.22 [0.00]	-12.02 [-11.80]
nitroethane	28.29	-0.22	-0.22 [-0.01]	-12.57 [-12.35]
N-methylaniline	5.96	-0.17	-0.19 [-0.02]	-9.47 [-9.30]
N,N-dimethylacetamide	37.781	-0.22	-0.23 [-0.01]	-29.14 [-28.92]
N,N-dimethylformamide	37.219	-0.22	-0.23 [-0.01]	-27.55 [-27.33]
n-nonane	1.9605	-0.08	-0.11 [-0.03]	-3.44 [-3.36]
n-octane	1.9406	-0.08	-0.11 [-0.03]	-3.57 [-3.49]
n-pentadecane	2.0333	-0.08	-0.12 [-0.03]	-3.01 [-2.93]
n-pentane	1.8371	-0.07	-0.10 [-0.03]	-4.11 [-4.04]
n-undecane	1.991	-0.08	-0.11 [-0.03]	-3.36 [-3.28]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-0.15	-0.18 [-0.03]	-5.69 [-5.53]
o-cresol	6.76	-0.18	-0.20 [-0.02]	11.39 [11.56]
o-dichlorobenzene	9.9949	-0.19	-0.21 [-0.02]	-4.38 [-4.19]
o-nitrotoluene	25.669	-0.22	-0.22 [-0.01]	-11.40 [-11.18]
o-xylene	2.5454	-0.11	-0.14 [-0.03]	-9.07 [-8.96]
pentanal	10	-0.19	-0.21 [-0.02]	-18.54 [-18.35]
pentanoicacid	2.6924	-0.11	-0.14 [-0.03]	10.39 [10.51]
pentylamine	4.201	-0.15	-0.18 [-0.03]	-16.57 [-16.43]
pentylethanoate	4.7297	-0.15	-0.18 [-0.03]	-18.60 [-18.45]
perfluorobenzene	2.029	-0.08	-0.12 [-0.03]	-4.05 [-3.97]
p-isopropyltoluene	2.2322	-0.09	-0.13 [-0.03]	-10.22 [-10.12]
propanal	18.5	-0.21	-0.22 [-0.01]	-18.78 [-18.57]
propanoicacid	3.44	-0.13	-0.16 [-0.03]	10.30 [10.44]
propanonitrile	29.324	-0.22	-0.22 [-0.01]	-14.18 [-13.96]
propylamine	4.9912	-0.16	-0.18 [-0.02]	-16.69 [-16.52]
propylethanoate	5.5205	-0.17	-0.19 [-0.02]	-18.70 [-18.53]
p-xylene	2.2705	-0.10	-0.13 [-0.03]	-9.24 [-9.15]
pyridine	12.978	-0.20	-0.21 [-0.01]	-20.79 [-20.59]
sec-butylbenzene	2.3446	-0.10	-0.13 [-0.03]	-9.00 [-8.90]
tert-butylbenzene	2.3447	-0.10	-0.13 [-0.03]	-9.06 [-8.96]
tetrachloroethene	2.268	-0.09	-0.13 [-0.03]	-3.49 [-3.40]
tetrahydrothiophene-S,S-dioxide	43.962	-0.22	-0.23 [-0.01]	-29.23 [-29.01]
tetralin	2.771	-0.12	-0.15 [-0.03]	-9.61 [-9.49]
thiophene	2.727	-0.11	-0.14 [-0.03]	-8.79 [-8.68]
thiophenol	4.2728	-0.15	-0.18 [-0.03]	-4.13 [-3.98]
trans-decalin	2.1781	-0.09	-0.12 [-0.03]	-2.84 [-2.75]
tributylphosphate	8.1781	-0.18	-0.20 [-0.02]	-45.67 [-45.49]
trichloroethene	3.422	-0.13	-0.16 [-0.03]	-0.69 [-0.55]
triethylamine	2.3832	-0.10	-0.13 [-0.03]	-30.94 [-30.84]
xylenemixture	2.3879	-0.10	-0.13 [-0.03]	-9.17 [-9.07]
Z-1,2-dichloroethene	9.2	-0.19	-0.20 [-0.02]	0.23 [0.41]

Table 5. Calculated standard state (298.15 K, 1 mol $L^{-1} \rightarrow$ 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for water (H_2O) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_o$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-17.13	-17.37 [-0.24]	e[a] [e]
methanol	32.613	-17.06	-17.32 [-0.26]	-30.82 [-13.77]
ethanol	24.852	-16.79	-17.13 [-0.34]	-30.13 [-13.34]
isoquinoline	11	-15.43	-16.12 [-0.69]	-15.78 [-0.35]
quinoline	9.16	-14.95	-15.76 [-0.80]	-15.33 [-0.38]
chloroform	4.7113	-12.47	-13.76 [-1.29]	-17.19 [-4.72]
diethylether	4.24	-11.94	-13.31 [-1.37]	-15.51 [-3.57]
dichloromethane	8.93	-14.88	-15.70 [-0.82]	-17.37 [-2.48]
dichloroethane	10.125	-15.22	-15.96 [-0.74]	-19.03 [-3.81]
carbontetrachloride	2.228	-7.72	-9.36 [-1.64]	-9.93 [-2.21]
benzene	2.2706	-7.87	-9.51 [-1.64]	-10.66 [-2.79]
toluene	2.3741	-8.22	-9.86 [-1.64]	-10.73 [-2.51]
chlorobenzene	5.6968	-13.32	-14.47 [-1.14]	-14.61 [-1.28]
nitromethane	36.562	-17.15	-17.38 [-0.23]	-19.27 [-2.12]
heptane	1.9113	-6.45	-8.02 [-1.58]	-8.33 [-1.89]
cyclohexane	2.0165	-6.90	-8.51 [-1.61]	-8.29 [-1.39]
aniline	6.8882	-14.05	-15.05 [-1.00]	-20.46 [-6.41]
acetone	20.493	-16.55	-16.96 [-0.40]	-20.56 [-4.01]
tetrahydrofuran	7.4257	-14.31	-15.26 [-0.95]	-16.98 [-2.66]
dimethylsulfoxide	46.826	-17.32	-17.50 [-0.18]	-19.96 [-2.64]
n-octanol	9.8629	-15.15	-15.91 [-0.76]	-26.40 [-11.25]
1,1,1-trichloroethane	7.0826	-14.15	-15.13 [-0.98]	-15.89 [-1.74]
1,1,2-trichloroethane	7.1937	-14.21	-15.18 [-0.97]	-18.60 [-4.39]
1,2,4-trimethylbenzene	2.3653	-8.19	-9.83 [-1.64]	-10.54 [-2.35]
1,2-dibromoethane	4.9313	-12.69	-13.94 [-1.25]	-15.48 [-2.79]
1,2-ethanediol	40.245	-17.22	-17.43 [-0.21]	-26.81 [-9.59]
1,4-dioxane	2.2099	-7.66	-9.29 [-1.64]	-11.07 [-3.41]
1-bromo-2-methylpropane	7.7792	-14.47	-15.38 [-0.91]	-15.95 [-1.48]
1-bromooctane	5.0244	-12.78	-14.01 [-1.24]	-13.85 [-1.08]
1-bromopentane	6.269	-13.71	-14.78 [-1.07]	-14.93 [-1.22]
1-bromopropane	8.0496	-14.57	-15.46 [-0.89]	-15.95 [-1.37]
1-butanol	17.332	-16.31	-16.78 [-0.46]	-28.93 [-12.62]
1-chlorohexane	5.9491	-13.50	-14.61 [-1.11]	-14.67 [-1.17]
1-chloropentane	6.5022	-13.84	-14.89 [-1.04]	-15.14 [-1.29]
1-chloropropane	8.3548	-14.69	-15.55 [-0.86]	-16.26 [-1.57]
1-decanol	7.5305	-14.36	-15.30 [-0.93]	-22.92 [-8.56]
1-fluorooctane	3.89	-11.48	-12.90 [-1.42]	-12.95 [-1.47]
1-heptanol	11.321	-15.50	-16.17 [-0.67]	-27.12 [-11.63]
1-hexanol	12.51	-15.72	-16.34 [-0.62]	-27.67 [-11.95]
1-hexene	2.0717	-7.13	-8.75 [-1.62]	-9.47 [-2.34]
1-hexyne	2.615	-8.94	-10.57 [-1.63]	-11.99 [-3.05]
1-iodobutane	6.173	-13.65	-14.73 [-1.08]	-15.01 [-1.37]
1-iodohexadecane	3.5338	-10.93	-12.42 [-1.49]	-11.95 [-1.02]
1-iodopentane	5.6973	-13.32	-14.47 [-1.14]	-14.62 [-1.30]
1-iodopropane	6.9626	-14.09	-15.08 [-0.99]	-15.39 [-1.29]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-16.74	-17.09 [-0.35]	-18.12 [-1.39]
1-nonanol	8.5991	-14.77	-15.62 [-0.85]	-23.83 [-9.05]
1-pentanol	15.13	-16.08	-16.61 [-0.53]	-28.45 [-12.37]
1-pentene	1.9905	-6.79	-8.39 [-1.60]	-9.41 [-2.62]
1-propanol	20.524	-16.56	-16.96 [-0.40]	-29.57 [-13.02]
2,2,2-trifluoroethanol	26.726	-16.87	-17.18 [-0.31]	-24.08 [-7.21]
2,2,4-trimethylpentane	1.9358	-6.56	-8.14 [-1.59]	-8.60 [-2.04]
2,4-dimethylpentane	1.8939	-6.37	-7.94 [-1.57]	-8.47 [-2.11]
2,4-dimethylpyridine	9.4176	-15.03	-15.82 [-0.79]	-16.78 [-1.75]
2,6-dimethylpyridine	7.1735	-14.20	-15.17 [-0.97]	-17.87 [-3.68]
2-bromopropane	9.361	-15.02	-15.81 [-0.79]	-14.94 [0.07]
2-butanol	15.944	-16.18	-16.68 [-0.50]	-28.79 [-12.62]
2-chlorobutane	8.393	-14.70	-15.56 [-0.86]	-16.33 [-1.63]
2-heptanone	11.658	-15.56	-16.22 [-0.66]	-16.74 [-1.18]
2-hexanone	14.136	-15.96	-16.52 [-0.56]	-18.89 [-2.93]
2-methoxyethanol	17.2	-16.30	-16.77 [-0.47]	-28.95 [-12.65]
2-methyl-1-propanol	16.777	-16.26	-16.74 [-0.48]	-29.10 [-12.84]
2-methyl-2-propanol	12.47	-15.71	-16.33 [-0.62]	-28.05 [-12.34]
2-methylpentane	1.89	-6.35	-7.92 [-1.57]	-8.51 [-2.16]
2-methylpyridine	9.9533	-15.18	-15.93 [-0.75]	-16.72 [-1.54]
2-nitropropane	25.654	-16.82	-17.15 [-0.33]	-18.37 [-1.55]
2-octanone	9.4678	-15.05	-15.83 [-0.78]	-16.30 [-1.26]
2-pentanone	15.2	-16.09	-16.62 [-0.53]	-19.23 [-3.14]
2-propanol	19.264	-16.47	-16.89 [-0.42]	-29.49 [-13.02]
2-propen-1-ol	19.011	-16.45	-16.88 [-0.43]	-29.33 [-12.88]
3-methylpyridine	11.645	-15.56	-16.22 [-0.66]	-16.75 [-1.19]
3-pentanone	16.78	-16.26	-16.74 [-0.48]	-19.23 [-2.97]
4-heptanone	12.257	-15.67	-16.30 [-0.63]	-16.97 [-1.30]
4-methyl-2-pentanone	12.887	-15.78	-16.38 [-0.60]	-18.93 [-3.15]
4-methylpyridine	11.957	-15.62	-16.26 [-0.64]	-16.76 [-1.14]
5-nonanone	10.6	-15.34	-16.05 [-0.71]	-16.55 [-1.21]
aceticacid	6.2528	-13.70	-14.77 [-1.07]	-19.16 [-5.47]
acetophenone	17.44	-16.32	-16.78 [-0.46]	-18.42 [-2.10]
2-chlorotoluene	6.7175	-13.97	-14.98 [-1.02]	-15.88 [-1.91]
anisole	4.2247	-11.93	-13.29 [-1.37]	-13.89 [-1.97]
benzaldehyde	18.22	-16.39	-16.83 [-0.44]	-18.49 [-2.10]
benzonitrile	25.592	-16.82	-17.15 [-0.33]	-18.29 [-1.47]
benzylalcohol	12.457	-15.71	-16.33 [-0.62]	-27.25 [-11.54]
bromobenzene	5.3954	-13.09	-14.27 [-1.18]	-14.35 [-1.26]
bromoethane	9.01	-14.91	-15.72 [-0.81]	-14.78 [0.13]
bromoform	4.2488	-11.95	-13.32 [-1.36]	-15.05 [-3.10]
butanal	13.45	-15.86	-16.45 [-0.58]	-18.58 [-2.71]
butanoicacid	2.9931	-9.88	-11.46 [-1.58]	-11.58 [-1.70]
butanone	18.246	-16.39	-16.83 [-0.44]	-19.39 [-3.00]
butanonitrile	24.291	-16.76	-17.11 [-0.34]	-18.70 [-1.94]
butylamine	4.6178	-12.38	-13.68 [-1.30]	-19.44 [-7.07]
butylethanoate	4.9941	-12.75	-13.99 [-1.24]	-15.63 [-2.88]
carbondisulfide	2.6105	-8.93	-10.55 [-1.63]	-10.38 [-1.45]
cis-1,2-dimethylcyclohexane	2.06	-7.08	-8.70 [-1.62]	-8.42 [-1.34]
cis-decalin	2.2139	-7.67	-9.30 [-1.64]	-8.36 [-0.69]
cyclohexanone	15.619	-16.14	-16.65 [-0.51]	-18.41 [-2.27]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-6.67	-8.26 [-1.59]	-8.33 [-1.67]
cyclopentanol	16.989	-16.28	-16.75 [-0.47]	-27.86 [-11.58]
cyclopentanone	13.58	-15.88	-16.46 [-0.58]	-18.13 [-2.24]
dibromomethane	7.2273	-14.22	-15.19 [-0.96]	-15.78 [-1.55]
dibutylether	3.0473	-10.00	-11.57 [-1.57]	-13.11 [-3.11]
diethylamine	3.5766	-11.00	-12.48 [-1.48]	-11.53 [-0.53]
diethylsulfide	5.723	-13.34	-14.48 [-1.14]	-15.77 [-2.43]
diiodomethane	5.32	-13.03	-14.23 [-1.19]	-12.00 [1.03]
diisopropylether	3.38	-10.66	-12.17 [-1.51]	-14.31 [-3.65]
dimethyldisulfide	9.6	-15.08	-15.86 [-0.77]	-14.77 [0.32]
diphenylether	3.73	-11.24	-12.70 [-1.45]	-14.32 [-3.08]
dipropylamine	2.9112	-9.69	-11.28 [-1.59]	-15.06 [-5.36]
E-1,2-dichloroethene	2.14	-7.40	-9.02 [-1.63]	-9.48 [-2.08]
E-2-pentene	2.051	-7.05	-8.66 [-1.61]	-9.55 [-2.51]
ethanethiol	6.667	-13.94	-14.96 [-1.02]	-16.08 [-2.14]
ethylbenzene	2.4339	-8.41	-10.05 [-1.64]	-10.68 [-2.27]
ethylethanoate	5.9867	-13.53	-14.63 [-1.10]	-16.45 [-2.92]
ethylmethanoate	8.331	-14.68	-15.55 [-0.87]	-15.46 [-0.78]
ethylphenylether	4.1797	-11.87	-13.24 [-1.37]	-14.15 [-2.28]
fluorobenzene	5.42	-13.11	-14.29 [-1.18]	-15.10 [-1.98]
formamide	108.94	-17.67	-17.75 [-0.08]	-25.07 [-7.40]
formicacid	51.1	-17.37	-17.54 [-0.17]	-22.68 [-5.31]
hexanoicacid	2.6	-8.90	-10.53 [-1.63]	-9.42 [-0.52]
iodobenzene	4.547	-12.30	-13.61 [-1.31]	-13.54 [-1.24]
iodoethane	7.6177	-14.40	-15.33 [-0.93]	-15.74 [-1.34]
iodomethane	6.865	-14.04	-15.04 [-1.00]	-15.18 [-1.13]
isopropylbenzene	2.3712	-8.21	-9.85 [-1.64]	-10.54 [-2.33]
m-cresol	12.44	-15.70	-16.33 [-0.62]	-24.01 [-8.31]
mesitylene	2.265	-7.85	-9.49 [-1.64]	-10.41 [-2.56]
methylbenzoate	6.7367	-13.98	-14.99 [-1.02]	-16.17 [-2.19]
methylbutanoate	5.5607	-13.22	-14.38 [-1.16]	-16.08 [-2.86]
methylcyclohexane	2.024	-6.93	-8.54 [-1.61]	-8.47 [-1.53]
methylethanoate	6.8615	-14.04	-15.04 [-1.00]	-16.74 [-2.69]
methylmethanoate	8.8377	-14.86	-15.68 [-0.82]	-15.42 [-0.57]
methylpropanoate	6.0777	-13.59	-14.68 [-1.09]	-16.40 [-2.81]
m-xylene	2.3478	-8.13	-9.77 [-1.64]	-10.52 [-2.38]
n-butylbenzene	2.36	-8.17	-9.81 [-1.64]	-10.25 [-2.08]
n-decane	1.9846	-6.77	-8.37 [-1.60]	-8.26 [-1.49]
n-dodecane	2.006	-6.86	-8.46 [-1.60]	-8.20 [-1.34]
n-hexadecane	2.0402	-7.00	-8.61 [-1.61]	-8.13 [-1.12]
n-hexane	1.8819	-6.31	-7.88 [-1.57]	-8.37 [-2.06]
nitrobenzene	34.809	-17.11	-17.36 [-0.24]	-18.17 [-1.06]
nitroethane	28.29	-16.93	-17.22 [-0.30]	-18.72 [-1.79]
N-methylaniline	5.96	-13.51	-14.62 [-1.11]	-20.04 [-6.53]
N,N-dimethylacetamide	37.781	-17.18	-17.40 [-0.23]	-20.58 [-3.41]
N,N-dimethylformamide	37.219	-17.16	-17.39 [-0.23]	-20.19 [-3.03]
n-nonane	1.9605	-6.66	-8.26 [-1.59]	-8.27 [-1.60]
n-octane	1.9406	-6.58	-8.17 [-1.59]	-8.31 [-1.73]
n-pentadecane	2.0333	-6.97	-8.58 [-1.61]	-8.14 [-1.16]
n-pentane	1.8371	-6.10	-7.65 [-1.55]	-8.40 [-2.31]
n-undecane	1.991	-6.79	-8.40 [-1.60]	-8.29 [-1.50]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-12.39	-13.69 [-1.30]	-13.58 [-1.19]
o-cresol	6.76	-13.99	-15.00 [-1.01]	-21.01 [-7.02]
o-dichlorobenzene	9.9949	-15.19	-15.94 [-0.75]	-14.06 [1.13]
o-nitrotoluene	25.669	-16.83	-17.15 [-0.32]	-17.59 [-0.77]
o-xylene	2.5454	-8.74	-10.38 [-1.63]	-10.95 [-2.21]
pentanal	10	-15.19	-15.94 [-0.75]	-16.13 [-0.94]
pentanoicacid	2.6924	-9.15	-10.77 [-1.62]	-10.02 [-0.87]
pentylamine	4.201	-11.90	-13.27 [-1.37]	-18.75 [-6.85]
pentylethanoate	4.7297	-12.49	-13.78 [-1.28]	-15.39 [-2.90]
perfluorobenzene	2.029	-6.95	-8.56 [-1.61]	-9.10 [-2.15]
p-isopropyltoluene	2.2322	-7.73	-9.37 [-1.64]	-10.30 [-2.57]
propanal	18.5	-16.41	-16.85 [-0.44]	-19.23 [-2.83]
propanoicacid	3.44	-10.76	-12.27 [-1.51]	-13.37 [-2.61]
propanonitrile	29.324	-16.96	-17.25 [-0.29]	-19.44 [-2.48]
propylamine	4.9912	-12.74	-13.99 [-1.24]	-20.13 [-7.39]
propylethanoate	5.5205	-13.19	-14.36 [-1.16]	-16.13 [-2.94]
p-xylene	2.2705	-7.87	-9.51 [-1.64]	-10.33 [-2.46]
pyridine	12.978	-15.79	-16.39 [-0.60]	-18.54 [-2.75]
sec-butylbenzene	2.3446	-8.12	-9.76 [-1.64]	-10.33 [-2.21]
tert-butylbenzene	2.3447	-8.12	-9.76 [-1.64]	-10.39 [-2.27]
tetrachloroethene	2.268	-7.86	-9.50 [-1.64]	-9.34 [-1.47]
tetrahydrothiophene-S,S-dioxide	43.962	-17.28	-17.48 [-0.19]	-18.06 [-0.78]
tetralin	2.771	-9.35	-10.96 [-1.61]	-11.17 [-1.82]
thiophene	2.727	-9.24	-10.86 [-1.61]	-11.40 [-2.16]
thiophenol	4.2728	-11.99	-13.34 [-1.36]	-14.95 [-2.97]
trans-decalin	2.1781	-7.54	-9.17 [-1.63]	-8.46 [-0.92]
tributylphosphate	8.1781	-14.62	-15.50 [-0.88]	-20.10 [-5.47]
trichloroethene	3.422	-10.73	-12.24 [-1.51]	-13.18 [-2.44]
triethylamine	2.3832	-8.25	-9.89 [-1.64]	-13.72 [-5.48]
xylenemixture	2.3879	-8.26	-9.90 [-1.64]	-10.61 [-2.35]
Z-1,2-dichloroethene	9.2	-14.97	-15.77 [-0.80]	-17.50 [-2.53]

[a] structure not converged.

Table 6. Calculated standard state (298.15 K, 1 mol L^{-1} → 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for carbon monoxide (CO) using the IEFPCM-UFF, CPCM, and SMD solvation models at the G4 level of theory. Values in brackets represent differences in ΔG_s° between the CPCM and SMD models and the IEFPCM-UFF model, respectively.

solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
acetonitrile	35.688	-1.16	-1.18 [-0.02]	13.55 [14.71]
methanol	32.613	-1.15	-1.18 [-0.03]	25.39 [26.54]
ethanol	24.852	-1.13	-1.17 [-0.03]	23.37 [24.50]
isoquinoline	11	-1.03	-1.10 [-0.07]	5.06 [6.10]
quinoline	9.16	-1.00	-1.08 [-0.08]	5.11 [6.11]
chloroform	4.7113	-0.82	-0.95 [-0.13]	16.01 [16.83]
diethylether	4.24	-0.78	-0.92 [-0.14]	10.22 [11.00]
dichloromethane	8.93	-0.99	-1.08 [-0.08]	14.16 [15.15]
dichloroethane	10.125	-1.02	-1.09 [-0.08]	15.29 [16.30]
carbontetrachloride	2.228	-0.49	-0.66 [-0.17]	11.23 [11.72]
benzene	2.2706	-0.50	-0.67 [-0.17]	11.84 [12.35]
toluene	2.3741	-0.53	-0.70 [-0.17]	12.04 [12.57]
chlorobenzene	5.6968	-0.88	-1.00 [-0.12]	12.35 [13.23]
nitromethane	36.562	-1.16	-1.18 [-0.02]	14.54 [15.70]
heptane	1.9113	-0.41	-0.57 [-0.16]	11.12 [11.53]
cyclohexane	2.0165	-0.44	-0.60 [-0.17]	12.02 [12.46]
aniline	6.8882	-0.93	-1.04 [-0.11]	23.12 [24.05]
acetone	20.493	-1.11	-1.16 [-0.04]	12.11 [13.22]
tetrahydrofuran	7.4257	-0.95	-1.05 [-0.10]	11.85 [12.80]
dimethylsulfoxide	46.826	-1.17	-1.19 [-0.02]	14.03 [15.20]
n-octanol	9.8629	-1.01	-1.09 [-0.08]	24.76 [25.77]
1,1,1-trichloroethane	7.0826	-0.94	-1.04 [-0.10]	10.87 [11.81]
1,1,2-trichloroethane	7.1937	-0.94	-1.04 [-0.10]	16.72 [17.66]
1,2,4-trimethylbenzene	2.3653	-0.53	-0.69 [-0.17]	12.64 [13.17]
1,2-dibromoethane	4.9313	-0.83	-0.96 [-0.13]	17.31 [18.14]
1,2-ethanediol	40.245	-1.16	-1.19 [-0.02]	35.29 [36.46]
1,4-dioxane	2.2099	-0.49	-0.66 [-0.17]	13.45 [13.94]
1-bromo-2-methylpropane	7.7792	-0.96	-1.06 [-0.09]	11.27 [12.23]
1-bromooctane	5.0244	-0.84	-0.97 [-0.13]	12.24 [13.08]
1-bromopentane	6.269	-0.91	-1.02 [-0.11]	11.82 [12.73]
1-bromopropane	8.0496	-0.97	-1.06 [-0.09]	11.38 [12.35]
1-butanol	17.332	-1.10	-1.14 [-0.05]	24.10 [25.19]
1-chlorohexane	5.9491	-0.89	-1.01 [-0.12]	11.52 [12.41]
1-chloropentane	6.5022	-0.92	-1.03 [-0.11]	11.24 [12.16]
1-chloropropane	8.3548	-0.98	-1.07 [-0.09]	10.50 [11.48]
1-decanol	7.5305	-0.96	-1.05 [-0.09]	25.12 [26.07]
1-fluorooctane	3.89	-0.75	-0.90 [-0.15]	11.26 [12.01]
1-heptanol	11.321	-1.04	-1.11 [-0.07]	24.63 [25.67]
1-hexanol	12.51	-1.05	-1.12 [-0.06]	24.43 [25.48]
1-hexene	2.0717	-0.45	-0.62 [-0.17]	10.83 [11.28]
1-hexyne	2.615	-0.57	-0.74 [-0.17]	15.26 [15.83]
1-iodobutane	6.173	-0.90	-1.02 [-0.11]	12.44 [13.34]
1-iodohexadecane	3.5338	-0.71	-0.87 [-0.15]	13.14 [13.85]
1-iodopentane	5.6973	-0.88	-1.00 [-0.12]	12.53 [13.41]
1-iodopropane	6.9626	-0.93	-1.04 [-0.10]	12.51 [13.45]

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solvent	$\varepsilon/\varepsilon_o$	IEFPCM-UFF	CPCM	SMD
1-nitropropane	23.73	-1.13	-1.16 [-0.04]	11.85 [12.98]
1-nonanol	8.5991	-0.98	-1.07 [-0.09]	24.95 [25.93]
1-pentanol	15.13	-1.08	-1.13 [-0.06]	24.26 [25.34]
1-pentene	1.9905	-0.43	-0.60 [-0.16]	10.44 [10.88]
1-propanol	20.524	-1.11	-1.16 [-0.04]	23.75 [24.86]
2,2,2-trifluoroethanol	26.726	-1.14	-1.17 [-0.03]	30.67 [31.81]
2,2,4-trimethylpentane	1.9358	-0.42	-0.58 [-0.16]	10.95 [11.36]
2,4-dimethylpentane	1.8939	-0.40	-0.57 [-0.16]	10.81 [11.21]
2,4-dimethylpyridine	9.4176	-1.00	-1.08 [-0.08]	12.76 [13.77]
2,6-dimethylpyridine	7.1735	-0.94	-1.04 [-0.10]	12.60 [13.54]
2-bromopropane	9.361	-1.00	-1.08 [-0.08]	11.01 [12.01]
2-butanol	15.944	-1.09	-1.14 [-0.05]	22.35 [23.44]
2-chlorobutane	8.393	-0.98	-1.07 [-0.09]	10.66 [11.64]
2-heptanone	11.658	-1.04	-1.11 [-0.07]	11.60 [12.64]
2-hexanone	14.136	-1.07	-1.13 [-0.06]	11.41 [12.48]
2-methoxyethanol	17.2	-1.09	-1.14 [-0.05]	22.60 [23.70]
2-methyl-1-propanol	16.777	-1.09	-1.14 [-0.05]	23.74 [24.83]
2-methyl-2-propanol	12.47	-1.05	-1.12 [-0.06]	21.30 [22.35]
2-methylpentane	1.89	-0.40	-0.56 [-0.16]	10.64 [11.04]
2-methylpyridine	9.9533	-1.01	-1.09 [-0.08]	12.61 [13.62]
2-nitropropane	25.654	-1.13	-1.17 [-0.03]	11.69 [12.83]
2-octanone	9.4678	-1.00	-1.08 [-0.08]	11.66 [12.66]
2-pentanone	15.2	-1.08	-1.13 [-0.06]	11.02 [12.10]
2-propanol	19.264	-1.11	-1.15 [-0.04]	21.95 [23.06]
2-propen-1-ol	19.011	-1.11	-1.15 [-0.04]	24.59 [25.69]
3-methylpyridine	11.645	-1.04	-1.11 [-0.07]	12.80 [13.84]
3-pentanone	16.78	-1.09	-1.14 [-0.05]	11.23 [12.32]
4-heptanone	12.257	-1.05	-1.12 [-0.07]	11.42 [12.47]
4-methyl-2-pentanone	12.887	-1.06	-1.12 [-0.06]	11.13 [12.19]
4-methylpyridine	11.957	-1.04	-1.11 [-0.07]	12.84 [13.89]
5-nonanone	10.6	-1.02	-1.10 [-0.08]	11.71 [12.73]
aceticacid	6.2528	-0.91	-1.02 [-0.11]	33.38 [34.29]
acetophenone	17.44	-1.10	-1.14 [-0.05]	13.60 [14.70]
2-chlorotoluene	6.7175	-0.93	-1.03 [-0.11]	13.29 [14.22]
anisole	4.2247	-0.78	-0.92 [-0.14]	13.11 [13.89]
benzaldehyde	18.22	-1.10	-1.15 [-0.04]	13.12 [14.22]
benzonitrile	25.592	-1.13	-1.17 [-0.03]	13.23 [14.36]
benzylalcohol	12.457	-1.05	-1.12 [-0.06]	24.66 [25.71]
bromobenzene	5.3954	-0.86	-0.99 [-0.12]	12.93 [13.79]
bromoethane	9.01	-1.00	-1.08 [-0.08]	10.96 [11.96]
bromoform	4.2488	-0.79	-0.92 [-0.14]	19.62 [20.40]
butanal	13.45	-1.06	-1.12 [-0.06]	11.12 [12.19]
butanoicacid	2.9931	-0.64	-0.80 [-0.16]	33.56 [34.20]
butanone	18.246	-1.10	-1.15 [-0.04]	11.02 [12.12]
butanonitrile	24.291	-1.13	-1.17 [-0.04]	11.33 [12.46]
butylamine	4.6178	-0.81	-0.95 [-0.13]	17.06 [17.87]
butylethanoate	4.9941	-0.84	-0.97 [-0.13]	11.57 [12.41]
carbondisulfide	2.6105	-0.57	-0.74 [-0.17]	14.16 [14.73]
cis-1,2-dimethylcyclohexane	2.06	-0.45	-0.62 [-0.17]	12.14 [12.59]
cis-decalin	2.2139	-0.49	-0.66 [-0.17]	13.26 [13.75]
cyclohexanone	15.619	-1.08	-1.14 [-0.05]	13.01 [14.09]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
cyclopentane	1.9608	-0.42	-0.59 [-0.17]	11.53 [11.95]
cyclopentanol	16.989	-1.09	-1.14 [-0.05]	23.71 [24.80]
cyclopentanone	13.58	-1.07	-1.12 [-0.06]	12.67 [13.74]
dibromomethane	7.2273	-0.95	-1.04 [-0.10]	16.67 [17.62]
dibutylether	3.0473	-0.65	-0.81 [-0.16]	11.89 [12.54]
diethylamine	3.5766	-0.72	-0.87 [-0.15]	39.93 [40.65]
diethylsulfide	5.723	-0.88	-1.00 [-0.12]	11.70 [12.58]
diiodomethane	5.32	-0.86	-0.98 [-0.12]	21.05 [21.91]
diisopropylether	3.38	-0.69	-0.85 [-0.16]	10.53 [11.22]
dimethyldisulfide	9.6	-1.01	-1.09 [-0.08]	13.28 [14.28]
diphenylether	3.73	-0.74	-0.88 [-0.15]	12.03 [12.77]
dipropylamine	2.9112	-0.63	-0.79 [-0.16]	14.51 [15.14]
E-1,2-dichloroethene	2.14	-0.47	-0.64 [-0.17]	14.99 [15.46]
E-2-pentene	2.051	-0.45	-0.61 [-0.17]	10.60 [11.05]
ethanethiol	6.667	-0.92	-1.03 [-0.11]	11.31 [12.23]
ethylbenzene	2.4339	-0.54	-0.71 [-0.17]	12.34 [12.88]
ethylethanoate	5.9867	-0.90	-1.01 [-0.11]	11.15 [12.05]
ethylmethanoate	8.331	-0.98	-1.07 [-0.09]	10.88 [11.86]
ethylphenylether	4.1797	-0.78	-0.92 [-0.14]	12.84 [13.62]
fluorobenzene	5.42	-0.87	-0.99 [-0.12]	11.16 [12.02]
formamide	108.94	-1.20	-1.21 [-0.01]	37.93 [39.12]
formicacid	51.1	-1.17	-1.19 [-0.02]	39.33 [40.51]
hexanoicacid	2.6	-0.57	-0.74 [-0.17]	34.01 [34.58]
iodobenzene	4.547	-0.81	-0.94 [-0.13]	13.93 [14.74]
iodoethane	7.6177	-0.96	-1.05 [-0.09]	12.48 [13.44]
iodomethane	6.865	-0.93	-1.03 [-0.10]	12.92 [13.85]
isopropylbenzene	2.3712	-0.53	-0.70 [-0.17]	12.33 [12.85]
m-cresol	12.44	-1.05	-1.12 [-0.06]	33.23 [34.29]
mesitylene	2.265	-0.50	-0.67 [-0.17]	12.41 [12.91]
methylbenzoate	6.7367	-0.93	-1.03 [-0.11]	13.53 [14.46]
methylbutanoate	5.5607	-0.87	-0.99 [-0.12]	11.45 [12.32]
methylcyclohexane	2.024	-0.44	-0.61 [-0.17]	11.80 [12.24]
methylethanoate	6.8615	-0.93	-1.03 [-0.10]	11.21 [12.15]
methylmethanoate	8.8377	-0.99	-1.08 [-0.09]	10.92 [11.91]
methylpropanoate	6.0777	-0.90	-1.01 [-0.11]	11.32 [12.22]
m-xylene	2.3478	-0.52	-0.69 [-0.17]	12.34 [12.87]
n-butylbenzene	2.36	-0.53	-0.69 [-0.17]	12.55 [13.08]
n-decane	1.9846	-0.43	-0.60 [-0.17]	11.75 [12.18]
n-dodecane	2.006	-0.44	-0.60 [-0.17]	12.02 [12.46]
n-hexadecane	2.0402	-0.45	-0.61 [-0.17]	12.39 [12.84]
n-hexane	1.8819	-0.40	-0.56 [-0.16]	10.80 [11.20]
nitrobenzene	34.809	-1.16	-1.18 [-0.03]	13.64 [14.80]
nitroethane	28.29	-1.14	-1.17 [-0.03]	12.72 [13.86]
N-methylaniline	5.96	-0.89	-1.01 [-0.12]	19.42 [20.31]
N,N-dimethylacetamide	37.781	-1.16	-1.18 [-0.02]	12.75 [13.91]
N,N-dimethylformamide	37.219	-1.16	-1.18 [-0.03]	12.87 [14.02]
n-nonane	1.9605	-0.42	-0.59 [-0.17]	11.59 [12.01]
n-octane	1.9406	-0.42	-0.58 [-0.16]	11.37 [11.79]
n-pentadecane	2.0333	-0.44	-0.61 [-0.17]	12.32 [12.76]
n-pentane	1.8371	-0.39	-0.55 [-0.16]	10.38 [10.76]
n-undecane	1.991	-0.43	-0.60 [-0.16]	12.05 [12.48]

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solvent	$\varepsilon/\varepsilon_\circ$	IEFPCM-UFF	CPCM	SMD
o-chlorotoluene	4.6331	-0.81	-0.95 [-0.13]	12.66 [13.48]
o-cresol	6.76	-0.93	-1.03 [-0.11]	31.73 [32.66]
o-dichlorobenzene	9.9949	-1.01	-1.09 [-0.08]	12.94 [13.96]
o-nitrotoluene	25.669	-1.13	-1.17 [-0.03]	13.84 [14.98]
o-xylene	2.5454	-0.56	-0.73 [-0.17]	12.52 [13.08]
pentanal	10	-1.01	-1.09 [-0.08]	11.41 [12.42]
pentanoicacid	2.6924	-0.59	-0.76 [-0.17]	33.81 [34.40]
pentylamine	4.201	-0.78	-0.92 [-0.14]	17.58 [18.36]
pentylethanoate	4.7297	-0.82	-0.95 [-0.13]	11.69 [12.51]
perfluorobenzene	2.029	-0.44	-0.61 [-0.17]	10.59 [11.04]
p-isopropyltoluene	2.2322	-0.50	-0.66 [-0.17]	12.34 [12.83]
propanal	18.5	-1.10	-1.15 [-0.05]	10.69 [11.79]
propanoicacid	3.44	-0.70	-0.86 [-0.15]	33.39 [34.09]
propanonitrile	29.324	-1.14	-1.17 [-0.03]	11.82 [12.96]
propylamine	4.9912	-0.84	-0.97 [-0.13]	16.67 [17.51]
propylethanoate	5.5205	-0.87	-0.99 [-0.12]	11.32 [12.19]
p-xylene	2.2705	-0.50	-0.67 [-0.17]	12.30 [12.80]
pyridine	12.978	-1.06	-1.12 [-0.06]	12.87 [13.93]
sec-butylbenzene	2.3446	-0.52	-0.69 [-0.17]	12.47 [12.99]
tert-butylbenzene	2.3447	-0.52	-0.69 [-0.17]	12.43 [12.95]
tetrachloroethene	2.268	-0.50	-0.67 [-0.17]	12.55 [13.06]
tetrahydrothiophene-S,S-dioxide	43.962	-1.17	-1.19 [-0.02]	16.93 [18.10]
tetralin	2.771	-0.60	-0.77 [-0.17]	13.42 [14.02]
thiophene	2.727	-0.60	-0.76 [-0.17]	12.65 [13.25]
thiophenol	4.2728	-0.79	-0.93 [-0.14]	16.82 [17.61]
trans-decalin	2.1781	-0.48	-0.65 [-0.17]	12.88 [13.36]
tributylphosphate	8.1781	-0.97	-1.06 [-0.09]	11.26 [12.23]
trichloroethene	3.422	-0.70	-0.85 [-0.15]	14.67 [15.37]
triethylamine	2.3832	-0.53	-0.70 [-0.17]	11.62 [12.15]
xylenemixture	2.3879	-0.53	-0.70 [-0.17]	12.38 [12.91]
Z-1,2-dichloroethene	9.2	-1.00	-1.08 [-0.08]	15.07 [16.06]

Table 7. Summary differences across 178 organic solvents between calculated standard state (298.15 K, 1 mol $L^{-1} \rightarrow$ 1 mol L^{-1}) Gibbs free energies of solvation (ΔG_s°; in kJ mol^{-1}) for various model combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) using the IEFPCM-UFF (PCM), CPCM, and SMD solvation models at the G4 level of theory. [a] mean signed deviation. [b] mean absolute deviation. [c] root mean squared deviation. [d] maximum absolute intra-solvent deviation.

	MSD[a]		MAD[b]		RMSD[c]		MADV[d]	
compound	PCM→CPCM	PCM→SMD	PCM→CPCM	PCM→SMD	PCM→CPCM	PCM→SMD	PCM→CPCM	PCM→SMD
N_2	-0.08	15.22	0.08	15.22	0.09	15.29	0.13	22.87
CO_2	-0.41	7.00	0.41	7.08	0.46	11.63	0.65	44.52
SO_2	-0.84	-2.76	0.84	6.50	0.92	7.63	1.30	26.79
O_2	-0.02	-9.04	0.02	10.64	0.02	13.16	0.03	45.49
H_2O	-1.04	-3.38	1.04	3.41	1.15	4.77	1.64	13.77
CO	-0.11	16.07	0.11	16.07	0.12	17.40	0.17	40.65

Using the IEFPCM-UFF ΔG_s° as an arbitrary datum for comparison, standard statistical metrics (mean signed deviation [MSD], mean absolute deviation [MAD], root mean squared deviation [RMSD], and maximum absolute intra-solvent deviation [MADV]) were generated for each compound with the CPCM and SMD models (Table 7). The IEFPCM-UFF and CPCM models yield similar ΔG_s° for all six compounds in each of the solvents considered, having MSD ranging between -0.02 and -1.04 kJ mol^{-1}, MAD<1.04 kJ mol^{-1}, RMSD<1.15 kJ mol^{-1}, and MADV<1.64 kJ mol^{-1}. In contrast, substantial ΔG_s° differences were observed between the IEFPCM-UFF and SMD models (and between the CPCM and SMD models), with MSD ranging between -9.04 and 16.07 kJ mol^{-1}, MAD up to 16.07 kJ mol^{-1}, RMSD up to 17.40 kJ mol^{-1}, and MADV up to 45.49 kJ mol^{-1}.

As expected, the IEFPCM-UFF and CPCM models displayed strong ΔG_s° correlations with the solvent dielectric constant ($\varepsilon/\varepsilon_\circ$) for each compound (Figure 1; note that the IEFPCM-UFF data plots behind the CPCM data points due to the similar ΔG_s° obtained by these two models), whereas the SMD model exhibits a significantly more variable (and potentially realistic, given the broad range of nonpolar aprotic, polar aprotic, and polar protic solvents under study) ΔG_s° relationship with $\varepsilon/\varepsilon_\circ$. Experimental ΔG_s° are available in the supporting compendia of Marenich et al. [19, 34] for water in various organic solvents (e.g., benzene, n-butyl acetate, carbon tetrachloride, chloroform, cyclohexane, diethyl ether, diisopropyl ether, ethyl acetate, ethylbenzene, n-hexadecane, isopropylbenzene, methylene chloride, n-octanol, sec-butanol, tetralin, toluene, tributylphosphate, and xylene). As discussed in ref. [19] during benchmarking of the SMD model, this model provides good agreement between experimental and estimated ΔG_s° for water in these solvents. Although there are literature reports on the experimental solvation free energies, solubilities, and Henry's law constants of the other combustion flue gases in selected organic solvents (see, e.g., ref. [35–55]), the lack of a complete experimental ΔG_s° database for all solute/solvent combinations presented herein under consistent standard-state conditions prevents the determination of rigorous error metrics.

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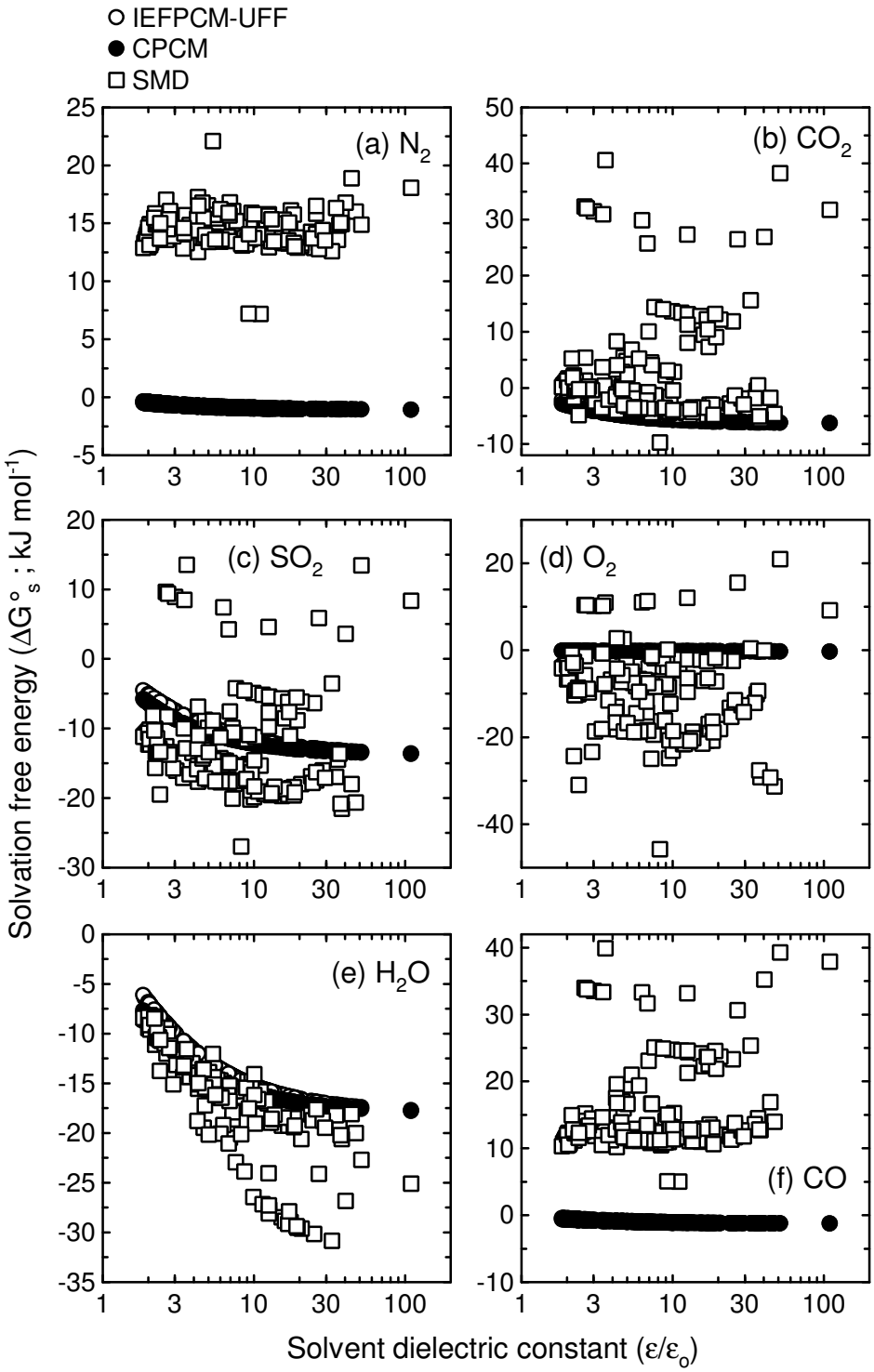

Figure 1: Relationships between estimated solvation free energies (ΔG°_s) at the Gaussian-4 (G4) level of theory and the solvent dielectric constant ($\varepsilon/\varepsilon_\circ$) for six model combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) in 178 organic solvents using the IEFPCM-UFF, CPCM, and SMD implicit solvation models.

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Supporting Information

Comparative study on the gas to solution phase solvation free energies of model combustion flue gas compounds (N_2, O_2, CO_2, H_2O, SO_2, and CO) in 178 organic solvents using the IEFPCM-UFF, CPCM, and SMD implicit solvent models at the Gaussian-4 (G4) level of theory

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Table S1. Gaussian-4 (G4) level of theory Gibbs free energies (in hartrees) at 298.15 K for N_2, CO_2, and SO_2 in the gas phase and solvents under consideration.

	N_2			CO_2			SO_2		
	IEFPCM-UFF	CPCM	SMD	IEFPCM-UFF	CPCM	SMD	IEFPCM-UFF	CPCM	SMD
air	-109.524945	-109.524945	-109.524945	-188.556615	-188.556615	-188.556615	-548.498828	-548.498828	-548.498828
acetonitrile	-109.525327	-109.525335	-109.519767	-188.558905	-188.558941	-188.556775	-548.503823	-548.503900	-548.504326
methanol	-109.525325	-109.525333	-109.520138	-188.558895	-188.558934	-188.550650	-548.503800	-548.503883	-548.500155
ethanol	-109.525319	-109.525329	-109.520031	-188.558859	-188.558909	-188.552087	-548.503717	-548.503824	-548.501225
isoquinoline	-109.525287	-109.525308	-109.522204	-188.558676	-188.558780	-188.558486	-548.503298	-548.503517	-548.504648
quinoline	-109.525276	-109.525301	-109.522189	-188.558613	-188.558733	-188.558428	-548.503154	-548.503407	-548.504564
chloroform	-109.525218	-109.525258	-109.519759	-188.558279	-188.558473	-188.554514	-548.502404	-548.502803	-548.502138
diethylether	-109.525206	-109.525248	-109.520166	-188.558208	-188.558414	-188.558132	-548.502246	-548.502668	-548.505534
dichloromethane	-109.525274	-109.525299	-109.519802	-188.558603	-188.558726	-188.555742	-548.503132	-548.503390	-548.503219
dichloroethane	-109.525282	-109.525305	-109.519390	-188.558649	-188.558760	-188.555511	-548.503235	-548.503469	-548.503082
carbontetrachloride	-109.525111	-109.525161	-109.519631	-188.557643	-188.557891	-188.556593	-548.501006	-548.501499	-548.503506
benzene	-109.525114	-109.525165	-109.519408	-188.557663	-188.557911	-188.556843	-548.501050	-548.501544	-548.504054
toluene	-109.525122	-109.525172	-109.519340	-188.557709	-188.557958	-188.556762	-548.501151	-548.501646	-548.503967
chlorobenzene	-109.525238	-109.525273	-109.519173	-188.558394	-188.558565	-188.556879	-548.502659	-548.503016	-548.504357
nitromethane	-109.525328	-109.525335	-109.519261	-188.558908	-188.558943	-188.556413	-548.503829	-548.503904	-548.504008
heptane	-109.525083	-109.525131	-109.519740	-188.557472	-188.557713	-188.556339	-548.500639	-548.501110	-548.502943
cyclohexane	-109.525093	-109.525142	-109.519383	-188.557533	-188.557778	-188.556088	-548.500771	-548.501252	-548.502802
aniline	-109.525255	-109.525286	-109.518535	-188.558492	-188.558642	-188.552758	-548.502880	-548.503194	-548.501682
acetone	-109.525313	-109.525326	-109.519958	-188.558828	-188.558887	-188.557864	-548.503644	-548.503772	-548.505667
tetrahydrofuran	-109.525261	-109.525290	-109.519544	-188.558526	-188.558668	-188.557937	-548.502959	-548.503256	-548.505648
dimethylsulfoxide	-109.525332	-109.525337	-109.518839	-188.558931	-188.558958	-188.558354	-548.503882	-548.503941	-548.506672
n-octanol	-109.525280	-109.525304	-109.519508	-188.558640	-188.558753	-188.551381	-548.503215	-548.503454	-548.500681
1,1,1-trichloroethane	-109.525257	-109.525287	-109.519779	-188.558505	-188.558652	-188.557391	-548.502910	-548.503217	-548.504731
1,1,2-trichloroethane	-109.525258	-109.525288	-109.519238	-188.558512	-188.558657	-188.554854	-548.502926	-548.503230	-548.502578
1,2,4-trimethylbenzene	-109.525121	-109.525172	-109.519131	-188.557705	-188.557954	-188.556658	-548.501142	-548.501637	-548.503927
1,2-dibromoethane	-109.525223	-109.525262	-109.518632	-188.558308	-188.558496	-188.554757	-548.502469	-548.502858	-548.502586
1,2-ethanediol	-109.525329	-109.525336	-109.518539	-188.558917	-188.558949	-188.546341	-548.503851	-548.503919	-548.497431
1,4-dioxane	-109.525109	-109.525160	-109.519020	-188.557634	-188.557882	-188.557249	-548.500988	-548.501479	-548.504777
1-bromo-2-methylpropane	-109.525264	-109.525292	-109.519643	-188.558547	-188.558684	-188.557308	-548.503005	-548.503292	-548.504674
1-bromooctane	-109.525225	-109.525263	-109.519290	-188.558320	-188.558506	-188.556805	-548.502495	-548.502879	-548.504093
1-bromopentane	-109.525247	-109.525280	-109.519442	-188.558445	-188.558605	-188.557037	-548.502775	-548.503109	-548.504370
1-bromopropane	-109.525267	-109.525294	-109.519605	-188.558561	-188.558695	-188.557268	-548.503038	-548.503317	-548.504633
1-butanol	-109.525308	-109.525322	-109.519748	-188.558795	-188.558865	-188.551794	-548.503569	-548.503718	-548.501023
1-chlorohexane	-109.525242	-109.525276	-109.519567	-188.558417	-188.558584	-188.557023	-548.502713	-548.503059	-548.504252
1-chloropentane	-109.525250	-109.525282	-109.519671	-188.558464	-188.558620	-188.557150	-548.502817	-548.503143	-548.504388
1-chloropropane	-109.525269	-109.525296	-109.519952	-188.558577	-188.558706	-188.557466	-548.503072	-548.503344	-548.504702
1-decanol	-109.525262	-109.525291	-109.519389	-188.558533	-188.558673	-188.551100	-548.502973	-548.503267	-548.500413
1-fluorooctane	-109.525195	-109.525239	-109.519689	-188.558146	-188.558361	-188.556906	-548.502108	-548.502548	-548.503953
1-heptanol	-109.525288	-109.525309	-109.519551	-188.558685	-188.558786	-188.551486	-548.503318	-548.503532	-548.500775
1-hexanol	-109.525294	-109.525313	-109.519627	-188.558715	-188.558808	-188.551597	-548.503386	-548.503583	-548.500872
1-hexene	-109.525098	-109.525147	-109.519859	-188.557563	-188.557810	-188.556690	-548.500836	-548.501321	-548.503430
1-hexyne	-109.525138	-109.525188	-109.519762	-188.557806	-188.558052	-188.554542	-548.501361	-548.501854	-548.501971
1-iodobutane	-109.525245	-109.525279	-109.519179	-188.558437	-188.558599	-188.557010	-548.502757	-548.503095	-548.504529
1-iodohexadecane	-109.525183	-109.525229	-109.518957	-188.558072	-188.558297	-188.556440	-548.501944	-548.502402	-548.503713
1-iodopentane	-109.525238	-109.525273	-109.519151	-188.558394	-188.558565	-188.556932	-548.502659	-548.503016	-548.504415
1-iodopropane	-109.525256	-109.525286	-109.519147	-188.558497	-188.558646	-188.557031	-548.502892	-548.503203	-548.504588
1-nitropropane	-109.525318	-109.525329	-109.519500	-188.558852	-188.558905	-188.557655	-548.503701	-548.503813	-548.505247
1-nonanol	-109.525271	-109.525298	-109.519445	-188.558588	-188.558715	-188.551240	-548.503099	-548.503365	-548.500545
1-pentanol	-109.525302	-109.525319	-109.519685	-188.558764	-188.558843	-188.551714	-548.503499	-548.503667	-548.500971
1-pentene	-109.525090	-109.525140	-109.520008	-188.557519	-188.557762	-188.556802	-548.500739	-548.501218	-548.503501

1-propanol	-109.525313	-109.525326	-109.519881	-188.558828	-188.558888	-188.551951	-548.503645	-548.503772	-548.501149
2,2,2-trifluoroethanol	-109.525321	-109.525331	-109.520066	-188.558870	-188.558917	-188.546510	-548.503742	-548.503842	-548.496573
2,2,4-trimethylpentane	-109.525085	-109.525134	-109.519796	-188.557487	-188.557728	-188.556432	-548.500671	-548.501145	-548.503063
2,4-dimethylpentane	-109.525081	-109.525129	-109.519855	-188.557462	-188.557701	-188.556451	-548.500616	-548.501086	-548.503045
2,4-dimethylpyridine	-109.525277	-109.525302	-109.519167	-188.558623	-188.558741	-188.558299	-548.503177	-548.503425	-548.506513
2,6-dimethylpyridine	-109.525258	-109.525288	-109.519235	-188.558511	-188.558656	-188.558290	-548.502923	-548.503228	-548.506452
2-bromopropane	-109.525277	-109.525301	-109.519748	-188.558621	-188.558739	-188.557494	-548.503172	-548.503421	-548.504895
2-butanol	-109.525304	-109.525320	-109.519866	-188.558777	-188.558852	-188.552980	-548.503527	-548.503687	-548.502055
2-chlorobutane	-109.525270	-109.525296	-109.519893	-188.558579	-188.558708	-188.557482	-548.503077	-548.503348	-548.504768
2-heptanone	-109.525290	-109.525310	-109.519635	-188.558694	-188.558793	-188.558245	-548.503339	-548.503548	-548.506083
2-hexanone	-109.525299	-109.525317	-109.519707	-188.558748	-188.558831	-188.558335	-548.503461	-548.503638	-548.506175
2-methoxyethanol	-109.525307	-109.525322	-109.519447	-188.558793	-188.558863	-188.553824	-548.503566	-548.503715	-548.503020
2-methyl-1-propanol	-109.525306	-109.525321	-109.519879	-188.558788	-188.558860	-188.551930	-548.503553	-548.503706	-548.501164
2-methyl-2-propanol	-109.525293	-109.525313	-109.520010	-188.558714	-188.558807	-188.553543	-548.503384	-548.503581	-548.502528
2-methylpentane	-109.525081	-109.525129	-109.519925	-188.557459	-188.557699	-188.556495	-548.500611	-548.501080	-548.503063
2-methylpyridine	-109.525281	-109.525304	-109.519216	-188.558643	-188.558755	-188.558226	-548.503222	-548.503459	-548.506372
2-nitropropane	-109.525320	-109.525330	-109.519566	-188.558864	-188.558913	-188.557764	-548.503728	-548.503832	-548.505370
2-octanone	-109.525278	-109.525302	-109.519609	-188.558625	-188.558742	-188.558195	-548.503181	-548.503428	-548.506025
2-pentanone	-109.525302	-109.525319	-109.519855	-188.558766	-188.558844	-188.558484	-548.503502	-548.503668	-548.506313
2-propanol	-109.525311	-109.525324	-109.520019	-188.558816	-188.558879	-188.553147	-548.503618	-548.503753	-548.502172
2-propen-1-ol	-109.525311	-109.525324	-109.519690	-188.558814	-188.558878	-188.551578	-548.503612	-548.503749	-548.500922
3-methylpyridine	-109.525290	-109.525310	-109.519130	-188.558694	-188.558792	-188.558087	-548.503338	-548.503547	-548.506215
3-pentanone	-109.525306	-109.525321	-109.519778	-188.558788	-188.558860	-188.558415	-548.503553	-548.503706	-548.506251
4-heptanone	-109.525293	-109.525312	-109.519700	-188.558709	-188.558803	-188.558327	-548.503373	-548.503573	-548.506173
4-methyl-2-pentanone	-109.525295	-109.525314	-109.519811	-188.558723	-188.558814	-188.558430	-548.503405	-548.503597	-548.506260
4-methylpyridine	-109.525291	-109.525311	-109.519113	-188.558702	-188.558798	-188.558070	-548.503356	-548.503560	-548.506198
5-nonanone	-109.525285	-109.525307	-109.519586	-188.558664	-188.558771	-188.558209	-548.503270	-548.503496	-548.506066
acetic acid	-109.525246	-109.525279	-109.519645	-188.558444	-188.558604	-188.545203	-548.502772	-548.503107	-548.495992
acetophenone	-109.525308	-109.525322	-109.518797	-188.558796	-188.558866	-188.557729	-548.503572	-548.503720	-548.505881
2-chlorotoluene	-109.525253	-109.525284	-109.518881	-188.558480	-188.558632	-188.557273	-548.502853	-548.503172	-548.505132
anisole	-109.525206	-109.525248	-109.518962	-188.558206	-188.558412	-188.557022	-548.502240	-548.502663	-548.504658
benzaldehyde	-109.525309	-109.525323	-109.518940	-188.558805	-188.558872	-188.557729	-548.503593	-548.503735	-548.505818
benzonitrile	-109.525320	-109.525330	-109.518900	-188.558864	-188.558912	-188.557496	-548.503727	-548.503832	-548.505464
benzylalcohol	-109.525293	-109.525313	-109.518928	-188.558714	-188.558807	-188.552307	-548.503383	-548.503581	-548.501734
bromobenzene	-109.525232	-109.525269	-109.518941	-188.558363	-188.558540	-188.556771	-548.502590	-548.502959	-548.504350
bromoethane	-109.525275	-109.525300	-109.519762	-188.558606	-188.558728	-188.557448	-548.503140	-548.503396	-548.504816
bromoform	-109.525206	-109.525248	-109.518355	-188.558210	-188.558415	-188.553427	-548.502249	-548.502671	-548.501429
butanal	-109.525297	-109.525315	-109.519810	-188.558735	-188.558822	-188.558238	-548.503432	-548.503617	-548.505954
butanoic acid	-109.525159	-109.525208	-109.519495	-188.557932	-188.558170	-188.544610	-548.501636	-548.502118	-548.495419
butanone	-109.525309	-109.525323	-109.519863	-188.558806	-188.558872	-188.558476	-548.503594	-548.503735	-548.506284
butanonitrile	-109.525318	-109.525329	-109.519713	-188.558856	-188.558907	-188.557973	-548.503709	-548.503819	-548.505602
butylamine	-109.525216	-109.525256	-109.519684	-188.558266	-188.558462	-188.555503	-548.502375	-548.502778	-548.503775
butylethanoate	-109.525224	-109.525263	-109.519654	-188.558316	-188.558503	-188.557828	-548.502486	-548.502872	-548.505396
carbondisulfide	-109.525138	-109.525188	-109.518449	-188.557804	-188.558051	-188.556096	-548.501357	-548.501851	-548.503589
cis-1,2-dimethylcyclohexane	-109.525097	-109.525146	-109.519331	-188.557557	-188.557803	-188.556074	-548.500822	-548.501307	-548.502824
cis-decalin	-109.525110	-109.525160	-109.518892	-188.557636	-188.557884	-188.555755	-548.500992	-548.501484	-548.502633
cyclohexanone	-109.525304	-109.525319	-109.519104	-188.558772	-188.558848	-188.557932	-548.503517	-548.503679	-548.505930
cyclopentane	-109.525088	-109.525137	-109.519577	-188.557501	-188.557744	-188.556229	-548.500702	-548.501179	-548.502887
cyclopentanol	-109.525307	-109.525322	-109.519203	-188.558791	-188.558862	-188.552615	-548.503560	-548.503711	-548.501719
cyclopentanone	-109.525297	-109.525315	-109.519228	-188.558737	-188.558824	-188.557906	-548.503437	-548.503621	-548.505810
dibromomethane	-109.525259	-109.525288	-109.518822	-188.558514	-188.558659	-188.555044	-548.502931	-548.503234	-548.502841
dibutylether	-109.525162	-109.525210	-109.519547	-188.557947	-188.558185	-188.557506	-548.501671	-548.502151	-548.504922
diethylamine	-109.525184	-109.525230	-109.519872	-188.558081	-188.558305	-188.541123	-548.501965	-548.502421	-548.493656
diethylsulfide	-109.525238	-109.525273	-109.519532	-188.558396	-188.558567	-188.557607	-548.502665	-548.503020	-548.505186

diiodomethane	-109.525231	-109.525268	-109.516519	-188.558354	-188.558534	-188.553993	-548.502572	-548.502943	-548.502189
diisopropylether	-109.525177	-109.525223	-109.520047	-188.558036	-188.558265	-188.557949	-548.501865	-548.502330	-548.505315
dimethyldisulfide	-109.525279	-109.525303	-109.518879	-188.558630	-188.558746	-188.557197	-548.503193	-548.503437	-548.505013
diphenylether	-109.525190	-109.525235	-109.519276	-188.558114	-188.558333	-188.557395	-548.502038	-548.502485	-548.505126
dipropylamine	-109.525155	-109.525204	-109.519651	-188.557907	-188.558147	-188.556739	-548.501581	-548.502066	-548.504792
E-1,2-dichloroethene	-109.525104	-109.525154	-109.519445	-188.557599	-188.557847	-188.554607	-548.500913	-548.501402	-548.501914
E-2-pentene	-109.525096	-109.525146	-109.519944	-188.557552	-188.557798	-188.556771	-548.500812	-548.501295	-548.503503
ethanethiol	-109.525252	-109.525284	-109.519662	-188.558476	-188.558629	-188.557570	-548.502844	-548.503165	-548.505054
ethylbenzene	-109.525126	-109.525176	-109.519236	-188.557734	-188.557983	-188.556669	-548.501206	-548.501701	-548.503884
ethylethanoate	-109.525242	-109.525276	-109.519821	-188.558421	-188.558586	-188.558007	-548.502720	-548.503065	-548.505566
ethylmethanoate	-109.525269	-109.525296	-109.519908	-188.558576	-188.558705	-188.557985	-548.503070	-548.503342	-548.505483
ethylphenylether	-109.525204	-109.525247	-109.519076	-188.558198	-188.558405	-188.557193	-548.502224	-548.502649	-548.504847
fluorobenzene	-109.525233	-109.525269	-109.519655	-188.558365	-188.558542	-188.557305	-548.502596	-548.502963	-548.504689
formamide	-109.525340	-109.525342	-109.518060	-188.558978	-188.558990	-188.544509	-548.503990	-548.504016	-548.495637
formic acid	-109.525333	-109.525338	-109.519271	-188.558938	-188.558963	-188.542026	-548.503897	-548.503952	-548.493692
hexanoic acid	-109.525137	-109.525187	-109.519333	-188.557800	-188.558047	-188.544285	-548.501348	-548.501842	-548.495141
iodobenzene	-109.525214	-109.525255	-109.518540	-188.558256	-188.558454	-188.556534	-548.502352	-548.502759	-548.504258
iodoethane	-109.525263	-109.525291	-109.519150	-188.558538	-188.558677	-188.557091	-548.502984	-548.503276	-548.504689
iodomethane	-109.525254	-109.525285	-109.518967	-188.558490	-188.558640	-188.556888	-548.502876	-548.503191	-548.504500
isopropylbenzene	-109.525122	-109.525172	-109.519248	-188.557708	-188.557957	-188.556676	-548.501148	-548.501643	-548.503879
m-cresol	-109.525293	-109.525313	-109.518969	-188.558713	-188.558806	-188.546187	-548.503382	-548.503580	-548.497060
mesitylene	-109.525114	-109.525164	-109.519219	-188.557660	-188.557909	-188.556722	-548.501044	-548.501538	-548.503965
methylbenzoate	-109.525253	-109.525284	-109.518845	-188.558481	-188.558633	-188.557454	-548.502856	-548.503174	-548.505401
methylbutanoate	-109.525235	-109.525271	-109.519702	-188.558380	-188.558554	-188.557898	-548.502629	-548.502991	-548.505477
methylcyclohexane	-109.525094	-109.525143	-109.519462	-188.557537	-188.557782	-188.556174	-548.500780	-548.501261	-548.502889
methylethanoate	-109.525254	-109.525285	-109.519806	-188.558490	-188.558640	-188.557985	-548.502876	-548.503190	-548.505532
methylmethanoate	-109.525273	-109.525299	-109.519908	-188.558599	-188.558723	-188.557930	-548.503123	-548.503383	-548.505381
methylpropanoate	-109.525244	-109.525277	-109.519755	-188.558429	-188.558593	-188.557951	-548.502738	-548.503080	-548.505521
m-xylene	-109.525120	-109.525170	-109.519237	-188.557698	-188.557946	-188.556681	-548.501126	-548.501621	-548.503897
n-butylbenzene	-109.525121	-109.525171	-109.519167	-188.557703	-188.557952	-188.556541	-548.501137	-548.501632	-548.503711
n-decane	-109.525090	-109.525139	-109.519494	-188.557515	-188.557759	-188.556149	-548.500732	-548.501210	-548.502815
n-dodecane	-109.525092	-109.525141	-109.519385	-188.557527	-188.557772	-188.556066	-548.500758	-548.501238	-548.502761
n-hexadecane	-109.525095	-109.525145	-109.519243	-188.557546	-188.557792	-188.555953	-548.500799	-548.501282	-548.502680
n-hexane	-109.525080	-109.525128	-109.519863	-188.557454	-188.557693	-188.556430	-548.500601	-548.501068	-548.502999
nitrobenzene	-109.525327	-109.525334	-109.518716	-188.558903	-188.558939	-188.557283	-548.503817	-548.503895	-548.505266
nitroethane	-109.525322	-109.525331	-109.519438	-188.558878	-188.558922	-188.557301	-548.503759	-548.503854	-548.504916
N-methylaniline	-109.525242	-109.525276	-109.518761	-188.558418	-188.558584	-188.554607	-548.502715	-548.503061	-548.503110
N,N-dimethylacetamide	-109.525328	-109.525335	-109.519252	-188.558911	-188.558945	-188.558697	-548.503837	-548.503909	-548.507007
N,N-dimethylformamide	-109.525328	-109.525335	-109.519209	-188.558910	-188.558944	-188.558512	-548.503833	-548.503907	-548.506738
n-nonane	-109.525088	-109.525137	-109.519556	-188.557501	-188.557744	-188.556198	-548.500702	-548.501178	-548.502849
n-octane	-109.525086	-109.525134	-109.519639	-188.557490	-188.557731	-188.556263	-548.500677	-548.501151	-548.502894
n-pentadecane	-109.525094	-109.525144	-109.519272	-188.557543	-188.557788	-188.555974	-548.500791	-548.501273	-548.502694
n-pentane	-109.525075	-109.525123	-109.520030	-188.557426	-188.557662	-188.556551	-548.500540	-548.501002	-548.503071
n-undecane	-109.525090	-109.525140	-109.519360	-188.557519	-188.557763	-188.556106	-548.500740	-548.501219	-548.502855
o-chlorotoluene	-109.525216	-109.525256	-109.519063	-188.558268	-188.558464	-188.556680	-548.502380	-548.502783	-548.504102
o-cresol	-109.525253	-109.525284	-109.518879	-188.558483	-188.558635	-188.546776	-548.502860	-548.503177	-548.497199
o-dichlorobenzene	-109.525281	-109.525304	-109.518922	-188.558644	-188.558756	-188.556761	-548.503225	-548.503462	-548.504354
o-nitrotoluene	-109.525320	-109.525330	-109.518653	-188.558864	-188.558913	-188.557108	-548.503728	-548.503832	-548.505019
o-xylene	-109.525134	-109.525184	-109.519166	-188.557779	-188.558027	-188.556670	-548.501303	-548.501798	-548.503941
pentanal	-109.525281	-109.525304	-109.519703	-188.558644	-188.558756	-188.558089	-548.503226	-548.503462	-548.505792
pentanoic acid	-109.525143	-109.525192	-109.519409	-188.557834	-188.558079	-188.544397	-548.501422	-548.501914	-548.495235
pentylamine	-109.525205	-109.525247	-109.519465	-188.558202	-188.558408	-188.555339	-548.502232	-548.502656	-548.503732
pentylethanoate	-109.525219	-109.525258	-109.519605	-188.558282	-188.558475	-188.557781	-548.502410	-548.502808	-548.505357
perfluorobenzene	-109.525094	-109.525143	-109.519934	-188.557540	-188.557785	-188.556574	-548.500786	-548.501268	-548.503202

p-isopropyltoluene	-109.525111	-109.525161	-109.519253	-188.557645	-188.557893	-188.556721	-548.501011	-548.501503	-548.503932
propanal	-109.525310	-109.525324	-109.519982	-188.558808	-188.558874	-188.558413	-548.503600	-548.503740	-548.506109
propanoic acid	-109.525179	-109.525225	-109.519550	-188.558050	-188.558277	-188.544812	-548.501896	-548.502359	-548.495586
propanonitrile	-109.525323	-109.525332	-109.519788	-188.558882	-188.558925	-188.557705	-548.503770	-548.503862	-548.505320
propylamine	-109.525224	-109.525263	-109.519830	-188.558316	-188.558503	-188.555678	-548.502485	-548.502872	-548.503915
propylethanoate	-109.525235	-109.525271	-109.519752	-188.558376	-188.558551	-188.557944	-548.502620	-548.502983	-548.505516
p-xylene	-109.525114	-109.525165	-109.519256	-188.557663	-188.557911	-188.556681	-548.501050	-548.501543	-548.503879
pyridine	-109.525295	-109.525314	-109.519092	-188.558725	-188.558815	-188.558034	-548.503409	-548.503600	-548.506161
sec-butylbenzene	-109.525120	-109.525170	-109.519200	-188.557696	-188.557945	-188.556602	-548.501123	-548.501617	-548.503786
tert-butylbenzene	-109.525120	-109.525170	-109.519209	-188.557696	-188.557945	-188.556627	-548.501123	-548.501618	-548.503823
tetrachloroethene	-109.525114	-109.525164	-109.519119	-188.557661	-188.557910	-188.556154	-548.501047	-548.501541	-548.503157
tetrahydrothiophene-S,S-dioxide	-109.525331	-109.525337	-109.517747	-188.558925	-188.558955	-188.557266	-548.503869	-548.503932	-548.505656
tetralin	-109.525147	-109.525197	-109.518819	-188.557861	-188.558105	-188.556506	-548.501481	-548.501971	-548.503925
thiophene	-109.525145	-109.525194	-109.519093	-188.557846	-188.558091	-188.556687	-548.501448	-548.501939	-548.504044
thiophenol	-109.525207	-109.525249	-109.518644	-188.558214	-188.558418	-188.555042	-548.502258	-548.502678	-548.502985
trans-decalin	-109.525107	-109.525157	-109.519036	-188.557618	-188.557866	-188.555878	-548.500954	-548.501445	-548.502728
tributylphosphate	-109.525268	-109.525295	-109.519905	-188.558568	-188.558700	-188.560289	-548.503053	-548.503329	-548.509072
trichloroethene	-109.525178	-109.525225	-109.519368	-188.558046	-188.558274	-188.555181	-548.501887	-548.502350	-548.502612
triethylamine	-109.525123	-109.525173	-109.519723	-188.557713	-188.557962	-188.558448	-548.501159	-548.501654	-548.506231
xylene mixture	-109.525123	-109.525173	-109.519220	-188.557715	-188.557964	-188.556679	-548.501163	-548.501659	-548.503908
Z-1,2-dichloroethene	-109.525276	-109.525301	-109.519576	-188.558614	-188.558734	-188.555416	-548.503157	-548.503410	-548.502969

Table S2. Gaussian-4 (G4) level of theory Gibbs free energies (in hartrees) at 298.15 K for O_2, H_2O, and CO in the gas phase and solvents under consideration.

	O_2			H_2O			CO		
	IEFPCM-UFF	CPCM	SMD	IEFPCM-UFF	CPCM	SMD	IEFPCM-UFF	CPCM	SMD
air	-150.298621	-150.298621	-150.298621	-76.415556	-76.415556	-76.415556	-113.308553	-113.308553	-113.308553
acetonitrile	-150.298705	-150.298706	-150.302436	-76.422081	-76.422172	n/c[a]	-113.308994	-113.309003	-113.303393
methanol	-150.298704	-150.298706	-150.298439	-76.422053	-76.422152	-76.427296	-113.308991	-113.309002	-113.298881
ethanol	-150.298703	-150.298705	-150.299522	-76.421951	-76.422079	-76.427033	-113.308984	-113.308997	-113.299652
isoquinoline	-150.298696	-150.298701	-150.300357	-76.421432	-76.421695	-76.421566	-113.308946	-113.308973	-113.306624
quinoline	-150.298693	-150.298699	-150.300356	-76.421252	-76.421558	-76.421396	-113.308933	-113.308965	-113.306606
chloroform	-150.298680	-150.298690	-150.297638	-76.420307	-76.420797	-76.422103	-113.308865	-113.308916	-113.302455
diethylether	-150.298678	-150.298688	-150.305513	-76.420105	-76.420625	-76.421464	-113.308851	-113.308905	-113.304660
dichloromethane	-150.298693	-150.298699	-150.298826	-76.421225	-76.421537	-76.422170	-113.308931	-113.308963	-113.303161
dichloroethane	-150.298695	-150.298700	-150.299295	-76.421354	-76.421636	-76.422806	-113.308940	-113.308970	-113.302730
carbontetrachloride	-150.298657	-150.298669	-150.300244	-76.418497	-76.419120	-76.419340	-113.308741	-113.308805	-113.304276
benzene	-150.298658	-150.298670	-150.302056	-76.418554	-76.419178	-76.419616	-113.308745	-113.308809	-113.304043
toluene	-150.298659	-150.298671	-150.301954	-76.418686	-76.419311	-76.419642	-113.308754	-113.308818	-113.303966
chlorobenzene	-150.298685	-150.298693	-150.300856	-76.420631	-76.421066	-76.421119	-113.308888	-113.308933	-113.303849
nitromethane	-150.298705	-150.298707	-150.302169	-76.422088	-76.422177	-76.422897	-113.308994	-113.309003	-113.303016
heptane	-150.298651	-150.298662	-150.300035	-76.418011	-76.418612	-76.418729	-113.308709	-113.308771	-113.304319
cyclohexane	-150.298653	-150.298665	-150.299857	-76.418185	-76.418797	-76.418714	-113.308720	-113.308783	-113.303976
aniline	-150.298688	-150.298696	-150.300173	-76.420909	-76.421290	-76.423349	-113.308908	-113.308948	-113.299746
acetone	-150.298702	-150.298705	-150.305503	-76.421861	-76.422014	-76.423387	-113.308977	-113.308993	-113.303942
tetrahydrofuran	-150.298690	-150.298697	-150.305999	-76.421008	-76.421368	-76.422022	-113.308915	-113.308953	-113.304038
dimethylsulfoxide	-150.298706	-150.298707	-150.310516	-76.422153	-76.422223	-76.423160	-113.308999	-113.309006	-113.303211
n-octanol	-150.298694	-150.298700	-150.299357	-76.421328	-76.421616	-76.425612	-113.308938	-113.308968	-113.299123
1,1,1-trichloroethane	-150.298689	-150.298696	-150.301277	-76.420947	-76.421319	-76.421610	-113.308911	-113.308949	-113.304414
1,1,2-trichloroethane	-150.298689	-150.298696	-150.299011	-76.420967	-76.421336	-76.422640	-113.308912	-113.308951	-113.302185
1,2,4-trimethylbenzene	-150.298659	-150.298671	-150.302445	-76.418675	-76.419300	-76.419571	-113.308753	-113.308817	-113.303738
1,2-dibromoethane	-150.298681	-150.298691	-150.299860	-76.420389	-76.420866	-76.421451	-113.308871	-113.308920	-113.301961
1,2-ethanediol	-150.298705	-150.298707	-150.298612	-76.422115	-76.422196	-76.425768	-113.308996	-113.309005	-113.295110
1,4-dioxane	-150.298656	-150.298669	-150.307857	-76.418472	-76.419095	-76.419772	-113.308739	-113.308804	-113.303430
1-bromo-2-methylpropane	-150.298691	-150.298697	-150.301511	-76.421066	-76.421414	-76.421631	-113.308919	-113.308955	-113.304260
1-bromooctane	-150.298682	-150.298691	-150.301296	-76.420422	-76.420893	-76.420832	-113.308873	-113.308922	-113.303892
1-bromopentane	-150.298687	-150.298695	-150.301382	-76.420777	-76.421184	-76.421241	-113.308899	-113.308941	-113.304051
1-bromopropane	-150.298691	-150.298698	-150.301468	-76.421107	-76.421446	-76.421630	-113.308922	-113.308957	-113.304220
1-butanol	-150.298700	-150.298704	-150.299433	-76.421769	-76.421946	-76.426575	-113.308971	-113.308989	-113.299375
1-chlorohexane	-150.298686	-150.298694	-150.301129	-76.420698	-76.421120	-76.421145	-113.308893	-113.308937	-113.304165
1-chloropentane	-150.298687	-150.298695	-150.301187	-76.420829	-76.421226	-76.421321	-113.308902	-113.308944	-113.304271
1-chloropropane	-150.298692	-150.298698	-150.301320	-76.421151	-76.421480	-76.421748	-113.308926	-113.308960	-113.304552
1-decanol	-150.298690	-150.298697	-150.299287	-76.421026	-76.421382	-76.424286	-113.308917	-113.308953	-113.298986
1-fluorooctane	-150.298675	-150.298686	-150.301181	-76.419929	-76.420471	-76.420487	-113.308839	-113.308895	-113.304263
1-heptanol	-150.298696	-150.298701	-150.299373	-76.421458	-76.421715	-76.425887	-113.308948	-113.308974	-113.299171
1-hexanol	-150.298697	-150.298702	-150.299411	-76.421542	-76.421778	-76.426093	-113.308954	-113.308978	-113.299250
1-hexene	-150.298654	-150.298666	-150.301034	-76.418271	-76.418888	-76.419162	-113.308726	-113.308790	-113.304428
1-hexyne	-150.298663	-150.298675	-150.299115	-76.418961	-76.419581	-76.420122	-113.308772	-113.308836	-113.302742
1-iodobutane	-150.298686	-150.298694	-150.301786	-76.420754	-76.421165	-76.421274	-113.308897	-113.308940	-113.303815
1-iodohexadecane	-150.298673	-150.298684	-150.301551	-76.419718	-76.420285	-76.420107	-113.308824	-113.308883	-113.303548
1-iodopentane	-150.298685	-150.298693	-150.301748	-76.420631	-76.421066	-76.421125	-113.308888	-113.308933	-113.303779
1-iodopropane	-150.298689	-150.298696	-150.301769	-76.420924	-76.421301	-76.421416	-113.308909	-113.308948	-113.303788
1-nitropropane	-150.298703	-150.298705	-150.303633	-76.421931	-76.422064	-76.422459	-113.308982	-113.308996	-113.304039
1-nonanol	-150.298692	-150.298699	-150.299318	-76.421183	-76.421505	-76.424631	-113.308928	-113.308961	-113.299051
1-pentanol	-150.298699	-150.298703	-150.299426	-76.421682	-76.421882	-76.426392	-113.308964	-113.308985	-113.299314
1-pentene	-150.298652	-150.298664	-150.301132	-76.418144	-76.418753	-76.419141	-113.308718	-113.308780	-113.304575

1-propanol	-150.298702	-150.298705	-150.299492	-76.421862	-76.422014	-76.426820	-113.308977	-113.308993	-113.299509
2,2,2-trifluoroethanol	-150.298703	-150.298706	-150.292670	-76.421981	-76.422100	-76.424728	-113.308986	-113.308999	-113.296871
2,2,4-trimethylpentane	-150.298651	-150.298663	-150.300106	-76.418053	-76.418657	-76.418831	-113.308712	-113.308774	-113.304384
2,4-dimethylpentane	-150.298650	-150.298662	-150.300122	-76.417981	-76.418580	-76.418783	-113.308707	-113.308769	-113.304437
2,4-dimethylpyridine	-150.298694	-150.298699	-150.308039	-76.421281	-76.421581	-76.421947	-113.308935	-113.308966	-113.303692
2,6-dimethylpyridine	-150.298689	-150.298696	-150.308104	-76.420963	-76.421333	-76.422364	-113.308912	-113.308950	-113.303755
2-bromopropane	-150.298693	-150.298699	-150.301814	-76.421275	-76.421576	-76.421248	-113.308935	-113.308966	-113.304361
2-butanol	-150.298700	-150.298703	-150.301265	-76.421717	-76.421908	-76.426522	-113.308967	-113.308987	-113.300040
2-chlorobutane	-150.298692	-150.298698	-150.301569	-76.421156	-76.421484	-76.421775	-113.308926	-113.308960	-113.304493
2-heptanone	-150.298696	-150.298701	-150.306463	-76.421483	-76.421734	-76.421933	-113.308950	-113.308976	-113.304136
2-hexanone	-150.298698	-150.298703	-150.306483	-76.421635	-76.421847	-76.422751	-113.308961	-113.308983	-113.304207
2-methoxyethanol	-150.298700	-150.298704	-150.305063	-76.421764	-76.421943	-76.426583	-113.308970	-113.308989	-113.299945
2-methyl-1-propanol	-150.298700	-150.298704	-150.299545	-76.421749	-76.421932	-76.426638	-113.308969	-113.308988	-113.299510
2-methyl-2-propanol	-150.298697	-150.298702	-150.302238	-76.421539	-76.421776	-76.426239	-113.308954	-113.308978	-113.300442
2-methylpentane	-150.298650	-150.298662	-150.300142	-76.417974	-76.418572	-76.418798	-113.308706	-113.308768	-113.304502
2-methylpyridine	-150.298694	-150.298700	-150.307401	-76.421337	-76.421623	-76.421925	-113.308939	-113.308969	-113.303752
2-nitropropane	-150.298703	-150.298706	-150.303923	-76.421964	-76.422088	-76.422554	-113.308985	-113.308998	-113.304099
2-octanone	-150.298694	-150.298700	-150.306484	-76.421287	-76.421585	-76.421766	-113.308935	-113.308966	-113.304112
2-pentanone	-150.298699	-150.298703	-150.306572	-76.421685	-76.421885	-76.422882	-113.308964	-113.308985	-113.304356
2-propanol	-150.298701	-150.298704	-150.301313	-76.421829	-76.421990	-76.426787	-113.308975	-113.308992	-113.300191
2-propen-1-ol	-150.298701	-150.298704	-150.299281	-76.421821	-76.421985	-76.426727	-113.308974	-113.308991	-113.299188
3-methylpyridine	-150.298696	-150.298701	-150.306819	-76.421482	-76.421733	-76.421935	-113.308950	-113.308976	-113.303679
3-pentanone	-150.298700	-150.298704	-150.306504	-76.421749	-76.421932	-76.422879	-113.308969	-113.308988	-113.304277
4-heptanone	-150.298697	-150.298702	-150.306515	-76.421525	-76.421765	-76.422021	-113.308953	-113.308978	-113.304205
4-methyl-2-pentanone	-150.298697	-150.298702	-150.306570	-76.421565	-76.421795	-76.422766	-113.308956	-113.308980	-113.304314
4-methylpyridine	-150.298697	-150.298701	-150.306799	-76.421505	-76.421750	-76.421938	-113.308951	-113.308977	-113.303661
5-nonanone	-150.298695	-150.298701	-150.306473	-76.421398	-76.421669	-76.421860	-113.308943	-113.308972	-113.304093
acetic acid	-150.298687	-150.298695	-150.294397	-76.420773	-76.421181	-76.422855	-113.308898	-113.308941	-113.295838
acetophenone	-150.298700	-150.298704	-150.305839	-76.421772	-76.421949	-76.422571	-113.308971	-113.308989	-113.303373
2-chlorotoluene	-150.298688	-150.298696	-150.304034	-76.420875	-76.421263	-76.421604	-113.308906	-113.308946	-113.303491
anisole	-150.298678	-150.298688	-150.303544	-76.420098	-76.420619	-76.420847	-113.308851	-113.308904	-113.303559
benzaldehyde	-150.298701	-150.298704	-150.304842	-76.421798	-76.421967	-76.422598	-113.308973	-113.308990	-113.303557
benzonitrile	-150.298703	-150.298706	-150.303916	-76.421963	-76.422088	-76.422522	-113.308985	-113.308998	-113.303514
benzylalcohol	-150.298697	-150.298702	-150.301032	-76.421538	-76.421775	-76.425935	-113.308954	-113.308978	-113.299161
bromobenzene	-150.298684	-150.298692	-150.301069	-76.420543	-76.420993	-76.421022	-113.308882	-113.308929	-113.303629
bromoethane	-150.298693	-150.298699	-150.301562	-76.421235	-76.421545	-76.421184	-113.308932	-113.308964	-113.304378
bromoform	-150.298678	-150.298688	-150.297535	-76.420109	-76.420628	-76.421288	-113.308852	-113.308905	-113.301081
butanal	-150.298698	-150.298702	-150.305721	-76.421598	-76.421820	-76.422632	-113.308958	-113.308981	-113.304316
butanoic acid	-150.298667	-150.298679	-150.294697	-76.419319	-76.419921	-76.419965	-113.308797	-113.308859	-113.295772
butanone	-150.298701	-150.298704	-150.306519	-76.421799	-76.421968	-76.422942	-113.308973	-113.308990	-113.304356
butanonitrile	-150.298703	-150.298705	-150.304415	-76.421941	-76.422072	-76.422679	-113.308983	-113.308997	-113.304239
butylamine	-150.298680	-150.298690	-150.304919	-76.420270	-76.420765	-76.422961	-113.308863	-113.308914	-113.302056
butylethanoate	-150.298682	-150.298691	-150.305707	-76.420411	-76.420884	-76.421509	-113.308873	-113.308922	-113.304145
carbondisulfide	-150.298663	-150.298675	-150.300790	-76.418957	-76.419576	-76.419508	-113.308772	-113.308836	-113.303161
cis-1,2-dimethylcyclohexane	-150.298654	-150.298666	-150.299846	-76.418253	-76.418869	-76.418763	-113.308725	-113.308788	-113.303930
cis-decalin	-150.298657	-150.298669	-150.299612	-76.418477	-76.419100	-76.418740	-113.308740	-113.308804	-113.303504
cyclohexanone	-150.298699	-150.298703	-150.306779	-76.421703	-76.421898	-76.422567	-113.308966	-113.308986	-113.303599
cyclopentane	-150.298652	-150.298664	-150.299958	-76.418095	-76.418702	-76.418730	-113.308714	-113.308777	-113.304163
cyclopentanol	-150.298700	-150.298704	-150.301044	-76.421757	-76.421937	-76.426167	-113.308970	-113.308988	-113.299524
cyclopentanone	-150.298698	-150.298702	-150.306316	-76.421605	-76.421825	-76.422460	-113.308959	-113.308981	-113.303727
dibromomethane	-150.298689	-150.298697	-150.299102	-76.420973	-76.421340	-76.421565	-113.308913	-113.308951	-113.302203
dibutylether	-150.298668	-150.298680	-150.305706	-76.419365	-76.419963	-76.420548	-113.308800	-113.308862	-113.304025
diethylamine	-150.298673	-150.298684	-150.294417	-76.419745	-76.420309	-76.419946	-113.308826	-113.308884	-113.293343
diethylsulfide	-150.298685	-150.298693	-150.304100	-76.420638	-76.421071	-76.421563	-113.308889	-113.308934	-113.304096

diiodomethane	-150.298683	-150.298692	-150.300462	-76.420520	-76.420974	-76.420128	-113.308880	-113.308927	-113.300534
diisopropylether	-150.298671	-150.298682	-150.305506	-76.419616	-76.420193	-76.421007	-113.308817	-113.308877	-113.304543
dimethyldisulfide	-150.298694	-150.298700	-150.303292	-76.421301	-76.421596	-76.421180	-113.308936	-113.308967	-113.303496
diphenylether	-150.298674	-150.298685	-150.302993	-76.419838	-76.420392	-76.421011	-113.308833	-113.308890	-113.303971
dipropylamine	-150.298666	-150.298678	-150.307505	-76.419248	-76.419854	-76.421291	-113.308792	-113.308854	-113.303027
E-1,2-dichloroethene	-150.298655	-150.298667	-150.298971	-76.418373	-76.418993	-76.419166	-113.308733	-113.308797	-113.302844
E-2-pentene	-150.298654	-150.298665	-150.301099	-76.418240	-76.418854	-76.419195	-113.308724	-113.308787	-113.304514
ethanethiol	-150.298688	-150.298696	-150.303103	-76.420865	-76.421254	-76.421679	-113.308905	-113.308945	-113.304245
ethylbenzene	-150.298660	-150.298672	-150.301975	-76.418759	-76.419383	-76.419624	-113.308759	-113.308823	-113.303853
ethylethanoate	-150.298686	-150.298694	-150.305744	-76.420708	-76.421128	-76.421821	-113.308894	-113.308937	-113.304306
ethylmethanoate	-150.298692	-150.298698	-150.304816	-76.421147	-76.421477	-76.421443	-113.308925	-113.308959	-113.304409
ethylphenylether	-150.298677	-150.298688	-150.304005	-76.420077	-76.420600	-76.420946	-113.308849	-113.308903	-113.303663
fluorobenzene	-150.298684	-150.298692	-150.301464	-76.420551	-76.421000	-76.421307	-113.308883	-113.308929	-113.304304
formamide	-150.298708	-150.298708	-150.295097	-76.422285	-76.422316	-76.425105	-113.309009	-113.309012	-113.294108
formic acid	-150.298706	-150.298707	-150.290606	-76.422172	-76.422237	-76.424193	-113.309000	-113.309007	-113.293572
hexanoic acid	-150.298663	-150.298675	-150.294625	-76.418945	-76.419565	-76.419144	-113.308771	-113.308835	-113.295599
iodobenzene	-150.298679	-150.298689	-150.301381	-76.420241	-76.420741	-76.420712	-113.308861	-113.308912	-113.303247
iodoethane	-150.298690	-150.298697	-150.301799	-76.421040	-76.421393	-76.421551	-113.308918	-113.308954	-113.303799
iodomethane	-150.298688	-150.298696	-150.301486	-76.420905	-76.421286	-76.421337	-113.308908	-113.308947	-113.303631
isopropylbenzene	-150.298659	-150.298671	-150.302103	-76.418683	-76.419307	-76.419572	-113.308754	-113.308818	-113.303858
m-cresol	-150.298697	-150.298702	-150.293997	-76.421537	-76.421774	-76.424701	-113.308954	-113.308978	-113.295895
mesitylene	-150.298657	-150.298670	-150.302516	-76.418547	-76.419170	-76.419522	-113.308744	-113.308809	-113.303826
methylbenzoate	-150.298688	-150.298696	-150.305594	-76.420879	-76.421266	-76.421715	-113.308906	-113.308946	-113.303399
methylbutanoate	-150.298684	-150.298693	-150.305710	-76.420592	-76.421034	-76.421680	-113.308886	-113.308931	-113.304192
methylcyclohexane	-150.298653	-150.298665	-150.299918	-76.418197	-76.418810	-76.418781	-113.308721	-113.308784	-113.304058
methylethanoate	-150.298688	-150.298696	-150.305661	-76.420904	-76.421286	-76.421930	-113.308908	-113.308947	-113.304282
methylmethanoate	-150.298693	-150.298699	-150.304730	-76.421214	-76.421528	-76.421430	-113.308930	-113.308963	-113.304395
methylpropanoate	-150.298686	-150.298694	-150.305701	-76.420731	-76.421147	-76.421803	-113.308895	-113.308938	-113.304241
m-xylene	-150.298659	-150.298671	-150.302122	-76.418654	-76.419278	-76.419562	-113.308752	-113.308816	-113.303852
n-butylbenzene	-150.298659	-150.298671	-150.301884	-76.418669	-76.419293	-76.419461	-113.308753	-113.308817	-113.303772
n-decane	-150.298652	-150.298664	-150.299892	-76.418134	-76.418743	-76.418703	-113.308717	-113.308780	-113.304079
n-dodecane	-150.298653	-150.298665	-150.299836	-76.418169	-76.418780	-76.418680	-113.308719	-113.308782	-113.303974
n-hexadecane	-150.298653	-150.298665	-150.299754	-76.418223	-76.418837	-76.418651	-113.308723	-113.308786	-113.303834
n-hexane	-150.298650	-150.298662	-150.300099	-76.417960	-76.418557	-76.418745	-113.308705	-113.308767	-113.304439
nitrobenzene	-150.298705	-150.298706	-150.303201	-76.422074	-76.422167	-76.422476	-113.308993	-113.309003	-113.303357
nitroethane	-150.298704	-150.298706	-150.303407	-76.422003	-76.422116	-76.422685	-113.308988	-113.309000	-113.303709
N-methylaniline	-150.298686	-150.298694	-150.302229	-76.420701	-76.421123	-76.423187	-113.308893	-113.308937	-113.301157
N,N-dimethylacetamide	-150.298705	-150.298707	-150.309720	-76.422098	-76.422184	-76.423395	-113.308995	-113.309004	-113.303696
N,N-dimethylformamide	-150.298705	-150.298707	-150.309116	-76.422093	-76.422181	-76.423247	-113.308994	-113.309004	-113.303653
n-nonane	-150.298652	-150.298663	-150.299932	-76.418094	-76.418701	-76.418705	-113.308714	-113.308777	-113.304140
n-octane	-150.298651	-150.298663	-150.299979	-76.418061	-76.418666	-76.418720	-113.308712	-113.308774	-113.304222
n-pentadecane	-150.298653	-150.298665	-150.299769	-76.418212	-76.418825	-76.418655	-113.308722	-113.308785	-113.303862
n-pentane	-150.298649	-150.298660	-150.300186	-76.417879	-76.418470	-76.418757	-113.308700	-113.308761	-113.304601
n-undecane	-150.298652	-150.298664	-150.299901	-76.418144	-76.418754	-76.418715	-113.308718	-113.308780	-113.303963
o-chlorotoluene	-150.298680	-150.298690	-150.300788	-76.420276	-76.420770	-76.420728	-113.308863	-113.308914	-113.303730
o-cresol	-150.298688	-150.298696	-150.294284	-76.420884	-76.421270	-76.423559	-113.308906	-113.308946	-113.296466
o-dichlorobenzene	-150.298694	-150.298700	-150.300291	-76.421342	-76.421627	-76.420912	-113.308939	-113.308969	-113.303623
o-nitrotoluene	-150.298703	-150.298706	-150.302962	-76.421965	-76.422088	-76.422257	-113.308985	-113.308998	-113.303280
o-xylene	-150.298662	-150.298674	-150.302074	-76.418886	-76.419508	-76.419726	-113.308767	-113.308831	-113.303785
pentanal	-150.298694	-150.298700	-150.305684	-76.421342	-76.421627	-76.421701	-113.308939	-113.308969	-113.304208
pentanoic acid	-150.298664	-150.298676	-150.294662	-76.419041	-76.419658	-76.419372	-113.308778	-113.308841	-113.295677
pentylamine	-150.298677	-150.298688	-150.304933	-76.420087	-76.420609	-76.422696	-113.308850	-113.308904	-113.301856
pentylethanoate	-150.298680	-150.298690	-150.305706	-76.420314	-76.420803	-76.421417	-113.308866	-113.308916	-113.304100
perfluorobenzene	-150.298653	-150.298665	-150.300165	-76.418205	-76.418818	-76.419023	-113.308722	-113.308785	-113.304519

p-isopropyltoluene	-150.298657	-150.298669	-150.302512	-76.418502	-76.419126	-76.419479	-113.308742	-113.308806	-113.303854
propanal	-150.298701	-150.298704	-150.305774	-76.421806	-76.421974	-76.422882	-113.308973	-113.308991	-113.304483
propanoic acid	-150.298672	-150.298683	-150.294697	-76.419656	-76.420230	-76.420649	-113.308820	-113.308879	-113.295836
propanonitrile	-150.298704	-150.298706	-150.304020	-76.422016	-76.422125	-76.422959	-113.308989	-113.309000	-113.304051
propylamine	-150.298682	-150.298691	-150.304976	-76.420410	-76.420883	-76.423223	-113.308873	-113.308922	-113.302203
propylethanoate	-150.298684	-150.298693	-150.305743	-76.420581	-76.421024	-76.421701	-113.308885	-113.308931	-113.304243
p-xylene	-150.298658	-150.298670	-150.302142	-76.418554	-76.419178	-76.419491	-113.308745	-113.308809	-113.303870
pyridine	-150.298698	-150.298702	-150.306539	-76.421571	-76.421800	-76.422619	-113.308956	-113.308980	-113.303650
sec-butylbenzene	-150.298659	-150.298671	-150.302048	-76.418649	-76.419274	-76.419492	-113.308751	-113.308816	-113.303805
tert-butylbenzene	-150.298659	-150.298671	-150.302073	-76.418650	-76.419274	-76.419514	-113.308751	-113.308816	-113.303818
tetrachloroethene	-150.298657	-150.298670	-150.299951	-76.418551	-76.419174	-76.419112	-113.308745	-113.308809	-113.303772
tetrahydrothiophene-S,S-dioxide	-150.298705	-150.298707	-150.309755	-76.422138	-76.422212	-76.422435	-113.308998	-113.309006	-113.302106
tetralin	-150.298665	-150.298677	-150.302281	-76.419119	-76.419732	-76.419812	-113.308783	-113.308846	-113.303443
thiophene	-150.298664	-150.298676	-150.301970	-76.419076	-76.419691	-76.419899	-113.308780	-113.308844	-113.303733
thiophenol	-150.298678	-150.298688	-150.300193	-76.420121	-76.420638	-76.421252	-113.308852	-113.308906	-113.302146
trans-decalin	-150.298656	-150.298668	-150.299703	-76.418428	-76.419049	-76.418780	-113.308737	-113.308801	-113.303647
tributylphosphate	-150.298691	-150.298698	-150.316016	-76.421126	-76.421460	-76.423210	-113.308924	-113.308958	-113.304264
trichloroethene	-150.298672	-150.298683	-150.298882	-76.419644	-76.420219	-76.420575	-113.308819	-113.308878	-113.302964
triethylamine	-150.298659	-150.298671	-150.310404	-76.418697	-76.419322	-76.420783	-113.308755	-113.308819	-113.304127
xylene mixture	-150.298659	-150.298672	-150.302112	-76.418703	-76.419328	-76.419598	-113.308755	-113.308819	-113.303836
Z-1,2-dichloroethene	-150.298693	-150.298699	-150.298535	-76.421257	-76.421562	-76.422221	-113.308933	-113.308965	-113.302815

1 structure not converged in solvent model.

END OF SUPPORTING INFORMATION