***Supporting Information for:***

# SM6T: A model to predict aqueous free energies of solvation as a function of temperature

***Adam C. Chamberlin, Christopher J. Cramer,* and Donald G. Truhlar****

*Department of Chemistry and Supercomputing Institute, 207 Pleasant St. SE, University of Minnesota, Minneapolis, MN 55455-0431*

*cramer@chem.umn.edu, truhlar@umn.edu

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**Table S1: The compounds in the database, the number of experimental points used for each compound, the minimum and maximum temperatures for which experimental data was available, and the minimum and maximum experimental free energies of solvation for each compound**

| | Number of Points | Minimum Experimental Temperature | Maximum Experimental Temperature | Minimum Experimental $\Delta G_S^\circ$ | Maximum Experimental $\Delta G_S^\circ$ |
|---|---|---|---|---|---|
| methane | 10 | 285.05 | 348.35 | 1.82 | 2.75 |
| ethane | 23 | 273.15 | 345.55 | 1.29 | 2.67 |
| propane | 14 | 283.15 | 347.25 | 1.61 | 2.91 |
| butane | 17 | 276.15 | 349.25 | 1.45 | 3.20 |
| pentane | 13 | 283.15 | 372.25 | 1.85 | 3.90 |
| hexane | 22 | 273.15 | 372.25 | 1.43 | 4.20 |
| heptane | 15 | 273.15 | 372.25 | 1.48 | 4.74 |
| octane | 12 | 288.15 | 372.25 | 1.47 | 5.40 |
| nonane | 7 | 288.15 | 372.25 | 2.37 | 5.77 |
| | | | | | |
| 2-methylbutane | 6 | 273.15 | 333.15 | 1.48 | 2.97 |
| 2,2-dimethylpropane | 4 | 298.15 | 353.15 | 2.50 | 4.87 |
| 2-methylpentane | 11 | 273.15 | 372.25 | 1.55 | 4.24 |
| 2,3-dimethylbutane | 10 | 273.15 | 372.25 | 1.34 | 3.98 |
| 2,2-dimethylhexane | 9 | 273 | 313 | 1.85 | 3.53 |
| 2,5-dimethylhexane | 9 | 273 | 313 | 1.91 | 3.46 |
| | | | | | |
| cyclopropane | 8 | 293.15 | 318.15 | 0.69 | 1.18 |
| cyclopentane | 12 | 298 | 372.25 | 1.13 | 2.55 |
| cyclohexene | 10 | 277.95 | 318.35 | -0.33 | 0.65 |
| cyclohexane | 7 | 287.95 | 318.35 | 0.66 | 1.95 |
| methylcyclohexane | 8 | 298.15 | 372.25 | 1.62 | 3.35 |
| cyclooctene | 9 | 273 | 313 | -0.35 | 0.80 |
| cyclooctane | 9 | 273 | 313 | 0.12 | 1.50 |
| ethylcyclohexane | 9 | 273 | 313 | 0.83 | 2.23 |
| cis-1,2-dimethylcyclohexane | 9 | 273 | 313 | 0.96 | 2.36 |
| trans-1,2-dimethylcyclohexane | 10 | 273 | 313 | 0.63 | 2.05 |
| trans-decalin | 5 | 283.15 | 303.15 | 0.62 | 1.25 |
| | | | | | |
| ethyne | 4 | 273.15 | 333.15 | -0.30 | 0.41 |
| ethene | 16 | 273 | 346.05 | 0.87 | 1.98 |
| propyne | 6 | 294.15 | 361.15 | -0.39 | 0.96 |
| propene | 14 | 273.15 | 323.15 | 0.40 | 2.76 |
| 2-methyl-1,3-butadiene | 4 | 293.15 | 333.15 | 0.66 | 1.23 |
| | | | | | |
| benzene | 78 | 275 | 373.14 | -1.45 | 0.07 |
| toluene | 53 | 273 | 353 | -1.60 | -0.13 |
| ethenylbenzene | 10 | 280.15 | 338.15 | -1.81 | -0.62 |
| o-xylene | 28 | 273.15 | 353 | -1.65 | 0.01 |
| m-xylene | 24 | 273 | 340.85 | -1.73 | -0.13 |
| p-xylene | 43 | 273.15 | 373.14 | -1.63 | 0.57 |

| | Number of Points | Minimum Experimental Temperature | Maximum Experimental Temperature | Minimum Experimental $\Delta G_S^\circ$ | Maximum Experimental $\Delta G_S^\circ$ |
|---|---|---|---|---|---|
| ethylbenzene | 83 | 273.15 | 373.14 | -1.58 | 0.60 |
| propylbenzene | 21 | 283 | 358.95 | -1.03 | 0.77 |
| cumene | 12 | 298.09 | 353.39 | -0.60 | 0.64 |
| 1,2,4-trimethylbenzene | 7 | 288 | 318 | -1.06 | -0.29 |
| 1,3,5-trimethylbenzene | 20 | 283 | 373.14 | -0.98 | 0.73 |
| naphthalene | 9 | 276.7 | 308.5 | -3.01 | -2.13 |
| tetralin | 5 | 283.15 | 303.15 | -1.93 | -1.34 |
| butylbenzene | 14 | 280.15 | 373.14 | -1.06 | 1.00 |
| 1-methylnaphthalene | 12 | 277.1 | 313.15 | -3.08 | -2.06 |
| 2-methylnaphthalene | 5 | 277.1 | 304 | -2.85 | -2.14 |
| acenaphthalene | 5 | 277.1 | 304 | -3.78 | -2.93 |
| anthracene | 4 | 284 | 304 | -4.14 | -3.45 |
| phenanthrene | 11 | 277.1 | 308.5 | -4.29 | -3.54 |
| 1-methylphenanthrene | 5 | 277.1 | 304 | -4.01 | -3.58 |
| pyrene | 5 | 277.1 | 304 | -4.72 | -4.13 |
| fluoranthene | 5 | 283 | 328 | -5.12 | -3.86 |
| | | | | | |
| water | 94 | 274.15 | 373.15 | -4.44 | -2.53 |
| methanol | 11 | 273 | 357.75 | -5.49 | -4.30 |
| ethanol | 10 | 273 | 333.15 | -5.64 | -4.20 |
| 1,2-ethanediol | 6 | 297.5 | 348.1 | -9.35 | -8.39 |
| 1-propanol | 5 | 273 | 313.15 | -5.59 | -4.25 |
| 2-propanol | 11 | 273 | 373.15 | -5.55 | -3.03 |
| 1-butanol | 58 | 273 | 373.15 | -5.51 | -3.02 |
| 2-butanol | 26 | 273 | 363.35 | -5.59 | -3.14 |
| 2-methyl-1-propanol | 26 | 273.15 | 372.19 | -5.32 | -2.92 |
| cyclopentanol | 8 | 273.15 | 363.65 | -6.40 | -3.92 |
| 1-pentanol | 19 | 273.15 | 373.15 | -5.53 | -2.58 |
| 2-pentanol | 9 | 298.15 | 363.45 | -4.32 | -2.47 |
| 3-pentanol | 13 | 273.15 | 363.15 | -5.16 | -2.43 |
| 2-methyl-1-butanol | 13 | 273.65 | 363.95 | -5.46 | -2.58 |
| 2-methyl-2-butanol | 13 | 273.65 | 363.35 | -4.99 | -2.39 |
| 2,2-dimethyl-1-propanol | 12 | 285.15 | 363.15 | -4.37 | -1.93 |
| 3-methyl-1-butanol | 18 | 283.25 | 363.15 | -4.90 | -2.63 |
| 3-methyl-2-butanol | 11 | 273.15 | 363.15 | -5.21 | -2.36 |
| phenol | 15 | 277.15 | 373.15 | -6.79 | -4.95 |
| cyclohexanol | 11 | 303.75 | 363.45 | -5.33 | -3.71 |
| 1-hexanol | 32 | 273.15 | 373.15 | -5.40 | -2.27 |
| 2-hexanol | 12 | 273.15 | 363.35 | -5.19 | -2.10 |
| 3-hexanol | 13 | 273.15 | 363.45 | -5.19 | -2.09 |
| 4-methyl-2-pentanol | 11 | 273.15 | 363.35 | -5.06 | -2.03 |
| 2-ethyl-1-butanol | 10 | 273.15 | 363.65 | -5.39 | -2.21 |
| benzylalcohol | 12 | 273.15 | 328.15 | -7.61 | -5.89 |
| 3-methylphenol | 26 | 283.15 | 371.65 | -6.26 | -4.71 |
| 2-methylphenol | 21 | 278.25 | 373.15 | -6.31 | -4.27 |
| 4-methylphenol | 16 | 278.2 | 373.15 | -6.77 | -4.69 |

| | Number of Points | Minimum Experimental Temperature | Maximum Experimental Temperature | Minimum Experimental $\Delta G_S^\circ$ | Maximum Experimental $\Delta G_S^\circ$ |
|---|---|---|---|---|---|
| cycloheptanol | 8 | 293.15 | 363.75 | -5.77 | -3.59 |
| 2-methylcyclohexanol | 9 | 273.15 | 353.25 | -5.47 | -3.04 |
| 3-methylcyclohexanol | 9 | 273.15 | 363.85 | -5.85 | -3.02 |
| 4-methylcyclohexanol | 10 | 273.15 | 363.65 | -6.10 | -3.09 |
| cyclohexylmethanol | 7 | 303.05 | 363.35 | -4.09 | -2.47 |
| 1-heptanol | 18 | 279.19 | 373.15 | -5.03 | -1.96 |
| 2-heptanol | 9 | 283.35 | 363.35 | -4.63 | -1.71 |
| 3-heptanol | 9 | 273.15 | 363.35 | -5.17 | -1.63 |
| 4-heptanol | 9 | 282.65 | 363.85 | -4.75 | -1.69 |
| 2,4-dimethyl-3-pentanol | 6 | 312.65 | 363.75 | -2.86 | -1.33 |
| 2-phenylethanol | 6 | 283.15 | 333.45 | -6.75 | -5.51 |
| cyclooctanol | 8 | 283.15 | 363.65 | -6.21 | -3.60 |
| 1-octanol | 5 | 293.96 | 342.46 | -4.17 | -1.86 |
| 2-octanol | 12 | 273.15 | 363.65 | -5.25 | -1.52 |
| 3-octanol | 9 | 283.15 | 363.25 | -4.56 | -1.41 |
| 2-ethyl-1-hexanol | 7 | 302.75 | 363.45 | -3.64 | -1.68 |
| 1-nonanol | 9 | 282.95 | 363.65 | -5.26 | -1.56 |
| 2-nonanol | 10 | 273.15 | 363.65 | -5.23 | -1.14 |
| | | | | | |
| formaldehyde | 9 | 283 | 318.15 | -6.94 | -6.29 |
| acetaldehyde | 10 | 273 | 313.15 | -4.03 | -3.06 |
| propanal | 5 | 283 | 318.15 | -3.82 | -2.93 |
| 2-oxo-propanal | 4 | 288 | 318.15 | -6.98 | -6.27 |
| butanal | 6 | 283 | 318.15 | -3.75 | -1.97 |
| pentanal | 6 | 283 | 318 | -3.63 | -1.15 |
| furfural | 42 | 273.15 | 371.05 | -5.79 | -4.42 |
| benzaldehyde | 18 | 273.15 | 363.15 | -4.84 | -3.10 |
| hexanal | 10 | 273.15 | 363.15 | -3.60 | -0.98 |
| heptanal | 12 | 273.15 | 363.15 | -3.66 | -0.82 |
| octanal | 5 | 283 | 318 | -3.33 | -1.56 |
| nonanal | 4 | 283 | 318 | -3.00 | -0.95 |
| 2-methylprop-2-enal | 11 | 278 | 333.15 | -3.24 | -2.09 |
| | | | | | |
| acetone | 13 | 273.66 | 333.15 | -4.38 | -3.17 |
| 2-butanone | 23 | 283 | 373.15 | -4.55 | -2.46 |
| cyclopentanone | 10 | 273.15 | 363.85 | -5.83 | -4.31 |
| 2-pentanone | 25 | 273.15 | 363.65 | -4.11 | -2.04 |
| 3-pentanone | 16 | 273.15 | 353.35 | -4.07 | -2.15 |
| 3-methyl-2-butanone | 10 | 273.15 | 362.15 | -4.06 | -1.92 |
| isopropylacetone | 9 | 273.15 | 348.15 | -3.53 | 0.15 |
| cyclohexanone | 10 | 273.15 | 363.85 | -5.74 | -3.70 |
| 2-hexanone | 15 | 273.15 | 364.65 | -4.13 | -1.76 |
| 4-methyl-2-pentanone | 18 | 273.15 | 363.55 | -3.87 | -1.49 |
| 3,3-dimethylbutanone | 12 | 282.65 | 363.35 | -3.18 | -1.22 |
| 2-heptanone | 14 | 273.15 | 363.65 | -3.99 | -1.34 |
| 4-heptanone | 15 | 273.15 | 363.65 | -3.99 | -1.34 |
| 5-methyl-2-hexanone | 10 | 273.15 | 362.85 | -3.90 | -1.33 |

| | Number of Points | Minimum Experimental Temperature | Maximum Experimental Temperature | Minimum Experimental $\Delta G_S^\circ$ | Maximum Experimental $\Delta G_S^\circ$ |
|---|---|---|---|---|---|
| 2,4-dimethyl-3-pentanone | 10 | 273.15 | 363.45 | -2.64 | -0.06 |
| 2-octanone | 9 | 273.15 | 364.15 | -4.67 | -1.06 |
| acetophenone | 7 | 288 | 318 | -5.21 | -4.09 |
| 2,6-dimethyl-4-heptanone | 10 | 273.15 | 363.85 | -3.15 | 0.03 |
| | | | | | |
| 1-methoxypropane | 6 | 273.15 | 298.15 | -2.35 | -1.64 |
| tetrahydrofuran | 5 | 293.15 | 343.15 | -3.58 | -2.72 |
| 2-methoxypropane | 5 | 283.15 | 298.15 | -2.32 | -1.90 |
| ethoxyethane | 34 | 273.15 | 355.15 | -2.72 | -0.66 |
| 2-methyltetrahydrofuran | 8 | 273.15 | 343.75 | -4.09 | -2.26 |
| 2-methoxy-2-methylpropane | 9 | 273.15 | 323.15 | -2.92 | -1.20 |
| 1-propxypropane | 4 | 273.15 | 298.15 | -2.10 | -1.17 |
| 2,5-dimethyltetrahydrofuran | 9 | 273.15 | 356.15 | -3.84 | -1.25 |
| 1-ethoxybutane | 10 | 273.15 | 363.85 | -2.70 | -0.13 |
| 2-Isopropoxypropane | 7 | 273.15 | 334.15 | -2.42 | 0.20 |
| methoxybenzene | 8 | 283.35 | 363.85 | -3.19 | -1.44 |
| 1-butoxybutane | 10 | 273.15 | 363.65 | -2.11 | 1.58 |
| | | | | | |
| methylethanoate | 14 | 278.15 | 345.05 | -3.68 | -2.95 |
| ethylformate | 10 | 278.15 | 348.65 | -2.93 | -2.25 |
| methylpropanoate | 14 | 273.15 | 343.35 | -3.60 | -2.10 |
| ethylethanoate | 32 | 273.15 | 343.65 | -3.64 | -2.16 |
| propylformate | 7 | 277.15 | 318.15 | -3.02 | -2.13 |
| isobutylformate | 7 | 273.15 | 333.55 | -2.84 | -1.36 |
| propylethanoate | 14 | 273.15 | 363.35 | -3.59 | -1.23 |
| 2-propylethanoate | 9 | 273.15 | 347.75 | -3.32 | -1.43 |
| 1-methylbutanoate | 10 | 273.15 | 363.65 | -3.49 | -1.21 |
| 1-ethylpropanoate | 9 | 273.15 | 353.45 | -3.54 | -1.49 |
| diethylcarbonate | 10 | 273.15 | 363.45 | -4.10 | -1.85 |
| dimethylmaleate | 10 | 273.15 | 363.65 | -7.16 | -5.30 |
| diethyloxalate | 6 | 273.15 | 322.85 | -6.43 | -4.73 |
| 1-ethylbutanoate | 10 | 273.15 | 363.65 | -3.28 | -0.76 |
| ethyl-2-methylproanoate | 10 | 273.15 | 363.75 | -3.01 | -0.41 |
| 1-butylethanoate | 13 | 273.15 | 363.65 | -3.50 | -0.96 |
| 2-methylpropylethanoate | 8 | 273.15 | 353.35 | -3.26 | -1.06 |
| 2-butylethanoate | 9 | 273.15 | 363.65 | -3.25 | -0.80 |
| tert-butylethanoate | 9 | 273.15 | 353.65 | -2.72 | -0.49 |
| pentylformate | 10 | 273.15 | 363.65 | -3.39 | -0.75 |
| 1-propylpropanoate | 10 | 273.15 | 363.65 | -3.39 | -0.67 |
| methylbenzoate | 9 | 273.15 | 363.65 | -4.70 | -2.56 |
| ethyl 3-methylbutanoate | 10 | 273.15 | 363.65 | -3.05 | -0.29 |
| 1-propylbutanoate | 8 | 273.15 | 363.65 | -3.19 | -0.53 |
| pentylethanoate | 8 | 273.15 | 353.25 | -3.53 | -1.00 |
| 3-methylbutylethanoate | 10 | 273.15 | 363.85 | -3.30 | -0.67 |
| methylsalicylate | 9 | 273.15 | 363.65 | -6.29 | -2.79 |
| diethylsuccinate | 10 | 273.15 | 363.85 | -7.43 | -4.46 |
| 1-butylbutyrate | 10 | 273.15 | 363.45 | -3.40 | -0.17 |

| | Number of Points | Minimum Experimental Temperature | Maximum Experimental Temperature | Minimum Experimental $\Delta G_S^\circ$ | Maximum Experimental $\Delta G_S^\circ$ |
|---|---|---|---|---|---|
| 2-methylpropyl-2-methylpropanoate | 10 | 273.15 | 363.35 | -4.63 | -2.67 |
| ethylbenzoate | 9 | 273.15 | 363.45 | -4.42 | -2.05 |
| octylmethanoate | 8 | 282.35 | 363.65 | -3.43 | -0.87 |
| | | | | | |
| formic acid | 4 | 277.78 | 308.64 | -7.09 | -6.74 |
| ethanoic acid | 4 | 277.78 | 308.64 | -7.20 | -6.68 |
| pentanoic acid | 9 | 277.78 | 308.64 | -6.92 | -6.08 |
| hexanoic acid | 13 | 273.15 | 333.15 | -7.04 | -5.16 |
| heptanoic acid | 9 | 273.15 | 333.15 | -7.73 | -5.17 |
| octanoic acid | 15 | 273.15 | 373.15 | -6.98 | -3.87 |
| nonanoic acid | 4 | 303.15 | 333.15 | -5.64 | -4.42 |

**Table S2: List of compounds for which experimental free energies of solvation were computed from Henry's Law constants, and the references and compilations of references from which they were obtained.**

| | Sources for Henry's Law Constants | Compilations | |
|---|---|---|---|
| 2,2-dimethylhexane | 1 | | |
| 2,5-dimethylhexane | 1 | | |
| cyclopentane | 2 | 3 | |
| cyclooctene | 1 | | |
| cyclooctane | 1 | | |
| ethylcyclohexane | 1 | | |
| cis-1,2-dimethylcyclohexane | 1 | | |
| trans-1,2-dimethylcyclohexane | 1 | | |
| trans-decalin | 4 | 3 | |
| | | | |
| ethene | 5 | | |
| benzene | 5-13 | 3 | 14 |
| toluene | 4-9,12,13,15-20 | 3 | 14 |
| o-xylene | 4,7,9,19,20 | 3 | |
| m-xylene | 4,5,7,9,20 | 3 | 14 |
| p-xylene | 2,4,5,7,9,20 | 3 | 14 |
| ethylbenzene | 4,7-9,13,16,20 | 3 | |
| propylbenzene | 4,16,20 | 3 | |
| 1,2,4-trimethylbenzene | 2,20 | 3 | |
| 1,3,5-trimethylbenzene | 4,13,20 | 3 | |
| naphthalene | 10 | 3 | |
| tetralin | 4 | 3 | |
| 1-methylnaphthalene | 21 | 3 | |
| 2-methylnaphthalene | 21 | 3 | |
| acenaphthalene | 21 | 3 | |
| anthracene | 10,21 | 3 | |
| phenanthrene | 10,21 | 3 | |
| 1-methylphenanthrene | 21 | 3 | |
| pyrene | 21 | 3 | |
| fluoranthene | 22 | 3 | |
| | | | |
| water | 23-27 | | |
| methanol | 28 | | 14 |
| ethanol | 28 | | 14 |
| 1,2-ethanediol | 29 | | |
| 1-propanol | 28 | | 14 |
| 2-propanol | 28 | | 14 |
| 1-butanol | 28 | | 14 |
| 2-butanol | 28 | | 14 |
| phenol | 30,31 | | |

| | Sources for Henry's Law Constants | Compilations |
|---|---|---|
| 3-methylphenol | 31,32 | |
| 2-methylphenol | 31,32 | |
| 4-methylphenol | 31,32 | |
| formaldehyde | 33,34 | 14 |
| acetaldehyde | 28,33,35 | 14 |
| propanal | 34 | 14 |
| 2-oxo-propanal | 33 | 14 |
| butanal | 34 | 14 |
| pentanal | 34 | 14 |
| benzaldehyde | 34,36 | 14 |
| heptanal | 34 | 14 |
| octanal | 34 | 14 |
| nonanal | 34 | 14 |
| 2-methylprop-2-enal | 36 | 14 |
| | | |
| acetone | 34,35,37 | 14 |
| 2-butanone | 34 | 14 |
| acetophenone | 36,37 | 14 |
| | | |
| tetrahydrofuran | 29 | |
| ethoxyethane | 15 | 14 |
| 2-methoxy-2-methylpropane | 7 | 14 |
| formic acid | 38 | 14 |
| ethanoic acid | 38 | 14 |
| pentanoic acid | 38,39 | 14 |

**Table S3: List of compounds for which experimental free energies of solvation were computed from vapor pressures and solubilities, and the references and compilations of solubilities from which they were obtained.**

| | Sources for Vapor Pressures | Sources for Solubilities | Compilations | |
|---|---|---|---|---|
| methane | 40 | 41 | | |
| ethane | 40 | 41-43 | | |
| propane | 40 | 41,43 | 44 | |
| butane | 40 | 41,45 | 44 | |
| pentane | 40 | 46-48 | 44 | |
| hexane | 49 | 46-48,50,51 | 44 | 52 |
| heptane | 49 | 46-48,50 | 44 | |
| octane | 49 | 47,48,51 | 44 | 52 |
| nonane | 49 | 47,48,51 | 44 | 52 |
| | | | | |
| 2-methylbutane | 40 | 50,53 | 44 | 52 |
| 2,2-dimethylpropane | 40 | 54 | 44 | |
| 2-methylpentane | 49 | 47,48,50 | 44 | |
| 2,3-dimethylbutane | 49 | 47,48,50 | 44 | |
| | | | | |
| cyclopropane | 40 | 55 | 44 | |
| cyclopentane | 40 | 47,48 | 44 | |
| cyclohexene | 56 | 57 | 44 | |
| cyclohexane | 40 | 57 | 44 | |
| methylcyclohexane | 49 | 47,48 | 44 | |
| | | | | |
| ethyne | 40 | 43 | 44 | |
| ethene | 40 | 41 | | |
| propyne | 40 | 58 | 44 | |
| propene | 40 | 43,59 | 44 | |
| 2-methyl-1,3-butadiene | 40 | 53 | | 52 |
| | | | | |
| benzene | 40 | 8,43,60-69 | 44 | |
| ethenylbenzene | 49 | 70 | 44 | |
| o-xylene | 49 | 50,71 | 44 | |
| m-xylene | 49 | 50,72 | 44 | |
| p-xylene | 49 | 50,71-73 | 44 | |
| ethylbenzene | 49 | 8,13,50,71,73-76 | 44 | |
| propylbenzene | 49 | 13,75 | 44 | |
| cumene | 49 | 77 | 44 | |
| 1,3,5-trimethylbenzene | 49 | 73 | 44 | |
| butylbenzene | 49 | 73,76 | 44 | |
| 1-methylnaphthalene | 49 | 78,79 | 44 | |
| | | | | |
| 1-butanol | 40,80 | 81-88 | 44 | |

| | Sources for Vapor Pressures | Sources for Solubilities | Compilations |
|---|---|---|---|
| 2-butanol | 40 | 81,89-91 | 44 |
| 2-methyl-1-propanol | 40,80 | 92 | 44 |
| cyclopentanol | 40 | 81 | |
| 1-pentanol | 40 | 84,93,94 | 44 |
| 2-pentanol | 40 | 93,94 | 44 |
| 3-pentanol | 40 | 93,94 | 44 |
| 2-methyl-1-butanol | 49 | 93,94 | 44 |
| 2-methyl-2-butanol | 40 | 93,94 | 44 |
| 2,2-dimethyl-1-propanol | 40 | 93,94 | 44 |
| 3-methyl-1-butanol | 40 | 93-96 | 44 |
| 3-methyl-2-butanol | 80 | 93,94 | 44 |
| cyclohexanol | 40,80 | 81,97,98 | 44 |
| 1-hexanol | 40 | 84,85,94,99 | 44 |
| 2-hexanol | 40 | 94,100 | 44 |
| 3-hexanol | 40 | 94,100 | 44 |
| 4-methyl-2-pentanol | 40 | 94,100 | 44 |
| 2-ethyl-1-butanol | 49 | 81 | |
| benzylalcohol | 49 | 81,101 | 44 |
| 3-methylphenol | 49,80 | 102-105 | 44 |
| 2-methylphenol | 49 | 97,105 | 44 |
| cycloheptanol | 40 | 81 | |
| 2-methylcyclohexanol | 49 | 81 | |
| 3-methylcyclohexanol | 49 | 81 | |
| 4-methylcyclohexanol | 49 | 81 | |
| cyclohexylmethanol | 49 | 81 | |
| 1-heptanol | 40 | 84,85,94,99 | 44 |
| 2-heptanol | 40 | 94 | 44 |
| 3-heptanol | 40 | 81 | |
| 4-heptanol | 40 | 81 | |
| 2,4-dimethyl-3-pentanol | 80 | 94 | 44 |
| 2-phenylethanol | 49 | 81 | |
| cyclooctanol | 40 | 81 | |
| 1-octanol | 40 | 106 | 44 |
| 2-octanol | 40,49 | 43,81,107 | 44 |
| 3-octanol | 40 | 81 | |
| 2-ethyl-1-hexanol | 40 | 94 | 44 |
| 1-nonanol | 49 | 81 | |
| 2-nonanol | 49 | 81 | |
| butanal | 56 | 108 | |
| furfural | 56 | 108-113 | 44 |
| benzaldehyde | 56 | 108 | |
| hexanal | 56 | 108 | |
| heptanal | 56 | 108 | |
| 2-methylprop-2-enal | 56 | 108 | |

| | Sources for Vapor Pressures | Sources for Solubilities | Compilations |
|---|---|---|---|
| 2-butanone | 40 | 43,114,115 | 44 |
| cyclopentanone | 56 | 116 | |
| 2-pentanone | 56 | 114-118 | 44 |
| 3-pentanone | 56 | 115,116,118 | 44 |
| 3-methyl-2-butanone | 56 | 116 | |
| isopropylacetone | 49 | 115,118,119 | 44 |
| cyclohexanone | 56 | 116 | |
| 2-hexanone | 56 | 115,116,118 | 44 |
| 4-methyl-2-pentanone | 56 | 115,116,118,119 | 44 |
| 3,3-dimethylbutanone | 56 | 115,116 | 44 |
| 2-heptanone | 56 | 115,116 | 44 |
| 4-heptanone | 56 | 116,118 | 44 |
| 5-methyl-2-hexanone | 56 | 116 | |
| 2,4-dimethyl-3-pentanone | 56 | 116 | |
| 2-octanone | 56 | 116 | |
| acetophenone | | | |
| 2,6-dimethyl-4-heptanone | 56 | 116 | |
| | | | |
| 1-methoxypropane | 40 | 120 | 44 |
| tetrahydrofuran | 49 | | |
| 2-methoxypropane | 40 | 120 | 44 |
| ethoxyethane | 40 | 43,96,121-124 | 44 |
| 2-methyltetrahydrofuran | 56 | 116 | |
| 2-methoxy-2-methylpropane | 56 | 116 | |
| 1-propxypropane | 40 | 120 | 44 |
| 2,5-dimethyltetrahydrofuran | 56 | 116 | |
| 1-ethoxybutane | 56 | 116 | |
| 2-Isopropoxypropane | 56 | 116 | |
| methoxybenzene | 56 | 116 | |
| 1-butoxybutane | 56 | 116 | |
| | | | |
| methylethanoate | 40 | 125,126 | 44 |
| ethylformate | 40 | 125 | 44 |
| methylpropanoate | 40,49 | 81,125 | 44 |
| ethylethanoate | 49 | 81,125,127-131 | 44 |
| propylformate | 49 | 125 | 44 |
| isobutylformate | 49 | 81 | |
| propylethanoate | 40,49 | 81 | |
| 2-propylethanoate | 40,49 | 81 | |
| 1-methylbutanoate | 49 | 81 | |
| 1-ethylpropanoate | 49 | 81 | |
| diethylcarbonate | 49 | 81 | |
| dimethylmaleate | 49 | 81 | |
| diethyloxalate | 49 | 81 | |

| | Sources for Vapor Pressures | Sources for Solubilities | Compilations |
|---|---|---|---|
| 1-ethylbutanoate | 49 | 81 | |
| ethyl-2-methylproanoate | 49 | 81 | |
| 1-butylethanoate | 40,49 | 81 | |
| 2-methylpropylethanoate | 49 | 81 | |
| 2-butylethanoate | 49 | 81 | |
| tert-butylethanoate | 49 | 81 | |
| pentylformate | 49 | 81 | |
| 1-propylpropanoate | 49 | 81 | |
| methylbenzoate | 49 | 81 | |
| ethyl 3-methylbutanoate | 49 | 81 | |
| 1-propylbutanoate | 49 | 81 | |
| pentylethanoate | 49 | 81 | |
| 3-methylbutylethanoate | 49 | 81 | |
| methylsalicylate | 49 | 81 | |
| diethylsuccinate | 49 | 81 | |
| 1-butylbutyrate | 49 | 81 | |
| 2-methylpropyl-2-methylpropanoate | 49 | 81 | |
| ethylbenzoate | 49 | 81 | |
| octylmethanoate | 49 | 81 | |
| | | | |
| hexanoic acid | 49 | 132-135 | 44 |
| heptanoic acid | 49 | 132,135 | 44 |
| octanoic acid | 49 | 53,132,135,136 | 44 |
| nonanoic acid | 49 | 136 | 44 |

**Table S4: List of compounds for which experimental free energies of solvation were computed from vapor pressures and activity coefficients at infinite dilution, and the references and compilations of solubilities from which they were obtained.**

| | Sources for Vapor Pressures | Sources for Activity Coefficients at Infinite Dilution | Compilation |
|---|---|---|---|
| benzene | 40 | 137 | 138 |
| methanol | 80 | 139,140 | 138 |
| ethanol | 80 | 139,141 | 138 |
| 1-propanol | 80 | 139,141 | 138 |
| 2-propanol | 80 | 140,142 | 138 |
| 1-butanol | 40,80 | 143-145 | 138 |
| 2-methyl-1-propanol | 40,80 | 15,143 | |
| cyclohexanol | 40,80 | 143 | |
| 3-methylphenol | 49,80 | 146 | 138 |
| acetone | 40 | 144,147 | 138 |
| 2-butanone | 40 | 143-145 | 138 |
| tetrahydrofuran | 49 | 143 | |
| propylethanoate | 40,49 | 146 | 138 |
| 2-propylethanoate | 40,49 | 146 | 138 |
| 1-butylethanoate | 40,49 | 146 | 138 |

**Table S5: Compounds for which experimental free energies of solvation at 298 K from the database used to parameterize SM6[148] were used.**

ethane
pentane
hexane
heptane
octane

2-methylbutane
2,2-dimethylpropane
2-methylpentane

cyclopropane
cyclopentane
methylcyclohexane
cis-1,2-dimethylcyclohexane

ethyne
ethene
propyne

o-xylene
m-xylene
ethylbenzene
naphthalene
anthracene

methanol
ethanol
1-propanol
2-propanol
1-butanol
3-methylphenol

acetaldehyde
propanal
butanal
pentanal
benzaldehyde
octanal

acetone
2-butanone
2-pentanone
3-pentanone
2-hexanone
2-heptanone
acetophenone

1-methoxypropane
2-methoxypropane
ethoxyethane

propylethanoate
1-butylethanoate

pentanoic acid
hexanoic acid
heptanoic acid
octanoic acid
nonanoic acid

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