



Minnesota Solvation (MNSOL) Database

An extensive and vetted database of free energies of solvation.



Applications

- Chemical engineering
- Drug development
- Developing solubility and bioavailability predictive models

Overview

The Minnesota Solvation Database consists of a collection of 3037 experimental free energies of solvation or transfer free energies for 790 unique solutes in 92 solvents (including water) and gas-phase M06-2X/MG3S optimized molecular geometries in Cartesian coordinates for the corresponding solutes. All of the 790 solutes in this database (541 neutrals and 249 singly-charged ions) contain at most the following elements: H, C, N, O, F, Si, P, S, Cl, Br, and I. User manual with detailed description of the dataset and example calculations is included.

Phase of Development

Database -- version 2012 (MNSol-v2012) -- available for download.

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Publications

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Category

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[*Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions*](#)

Journal of Physical Chemistry B, 113, 6378–6396 (2009)

[*Generalized Born Solvation Model SM12*](#)

Journal of Chemical Theory and Computation, 9, 609-620 (2013)

External Links

[AMSOL 7.1: Software to Calculate Free Energies of Solvation](#)

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- Commercial organizations must purchase the online license using the link provided on the right panel.