UNIVERSITY OF MINNESOTA
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Minnesota Solvation (MNSOL) Database

An extensive and vetted database of free energies of solvation.

Technology ID

2020-340

Category

Express License
Engineering & Physical Sciences/Chemicals
Life Sciences/Biologics
Life Sciences/Pharmaceuticals
Software & IT/Databases
Software & IT/Open Source

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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.

Researchers

Christopher J. Cramer, PhD
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Publications

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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