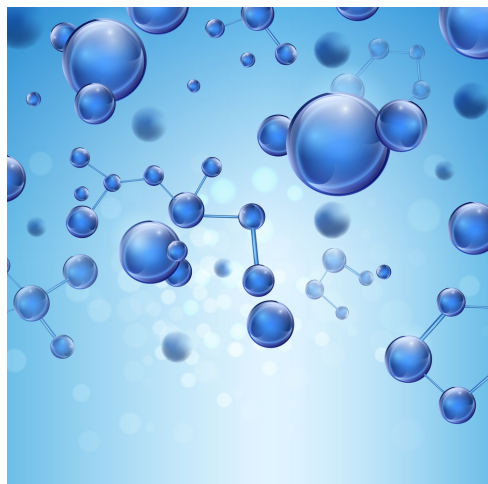




## AMSOL 7.1: Software to Calculate Free Energies of Solvation



### Technology ID

z05201

### Category

Express License

Engineering & Physical

Sciences/Chemicals

Software & IT/Algorithms

### Learn more



### Computational Chemistry, Molecular Solvation Software

AMSOL is a computational chemistry software program that calculates the free energy of a solvated molecule. The software application calculates the change in energy when molecules are dissolved in water or an organic solvent. The results may also be used to calculate partition coefficients and their logarithms (Log P). The SM1 - SM5.42R solvation models are used to calculate the free energies of solvation in water, the SM4 solvation model is used to calculate the free energies of solvation in alkanes, and the SM5.0 - SM5.42R solvation models are used for general organic solvents.

### CHARGE MODEL (CM) ALSO AVAILABLE

AMSOL can also be used to calculate partial atomic charges by the CM1A, CM1P, CM2/AM1, CM2/PM3, CM3/AM1, and CM3/PM3 charge models. These models are used to calculate partial atomic charges in the gas phase, in aqueous solution, or in general organic solvents. Partial atomic charges are important electrostatic descriptors and may be used in theoretical structure activity relations (not included).

[AMSOL Home Page](#)

### Commercial Distribution License

There are variabilities in the commercial license for AMSOL that are best addressed with a conversation. If you are interested in a commercial license with rights to distribute please contact us with your interests. A Marketing Technology Manager will contact you with further information.

**Researchers:** Donald Truhlar, Regents Professor, Chemistry Department, College of Science and Engineering  
Christopher J. Cramer, Distinguished McKnight University Professor, Chemistry Department, College of Science and Engineering