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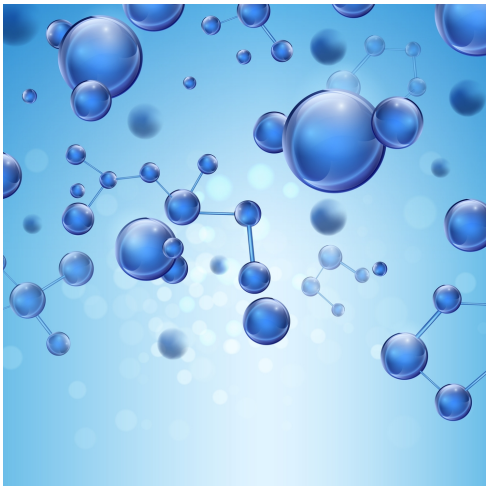
AMSOL 7.1: Software to Calculate Free Energies of Solvation



Technology ID

z05201

Category

Express License
Engineering & Physical Sciences/Chemicals
Software & IT/Algorithms

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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

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