

Russian Journal of Physical Chemistry A 2008 vol.82 N5, pages 704-708

A method for calculating the Gibbs energy of nonspecific solvation

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Abstract

A method for calculating the Gibbs energy of nonspecific solvation of nonelectrolytes was suggested. The new equation for the Gibbs energy of nonspecific solvation contains one solvent parameter that characterizes nonspecific solvent-solute interactions and two experimental Gibbs energies of solvation in two standard solvents. The method is applicable to a wide range of solutes and solvents. It was successfully used to describe some 800 Gibbs energies of solvation for systems without specific solvent-solute interactions. © 2008 MAIK Nauka.

<http://dx.doi.org/10.1134/S0036024408050026>
