عنوان مقاله:

Thermodynamic and Theoretical solvation parameters for 2-amino-4,5-dimethylthiophene-3-carboxamide(ADTC) in Ethanol and Mixed EtOH-H2O solvents

محل انتشار:

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خلاصه مقاله:

The molar solubility for 2-amino-4,5-dimethylthiophene-3-carboxamide (ADTC) in pure ethanol and mixed ethanol (EtOH)- water solvents were measured at five different temperatures, 293.15, 298.15, 303.15, 308.15, and 313.15 K in the used mixed solvents, the solubility were increase by increase in the mole fraction of ethanol in the mixtures and increase of temperature due to more salvation parameters. All the solvation and thermodynamic parameters for ADTC in mixed EtOH+ H2O solvents were evaluated like solubility products, Gibbs free energies, enthalpies and entropies of solvation and discussed. Theoretical calculations for (ADTC) were done quantum mechanically by using Gaussian on .set of calculations in ethanol for evaluating the different thermodynamic parameters

کلمات کلیدی:

Thermodynamic, Theoretical solvation, Dimethylthiophene-caboxamide

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