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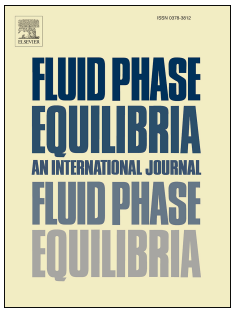

Solubility of 1-methyl-4-nitropyrazole in seventeen pure solvents at temperatures from 283.15□K to 323.15□K

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Solubility of 1-methyl-4-nitropyrazole in seventeen pure solvents at temperatures from 283.15 K to 323.15 K

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Abstract: Knowledge of solubility for 1-methyl-4-nitropyrazole (1-M-4-NP) in different solvents is important for its purification and further theoretical studies. In this paper, the solubility of 1-M-4-NP in toluene, 1,2-dichlorobenzene, water, methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 1-pentanol, 2-pentanol, methyl acetate, ethyl acetate, acetone, butanone, acetic acid and acetonitrile were determined at T = (283.15, 288.15, 293.15, 298.15, 303.15, 308.15, 313.15, 318.15 and 323.15) K under atmospheric pressure (P = 0.1 MPa) by a gravimetric method. The results showed that the solubility increases with rise of temperature in all selected solvents and the solubility in acetone increases fastest. In alcoholic solvents, the solubility decreases with the increasing in the number of carbon atoms in the alcohol. Additionally, melting temperature and fusion enthalpy of 1-M-4-NP were measured by differential scanning calorimetry (DSC). Besides, the solubility values were correlated by the modified Apelblat equation, the polynomial empirical equation, λh equation and NRTL model. Since the correlation coefficients (R^2) of the four models are greater than 0.9900 and the largest values of the root-mean-square was 7.00×10^{-2}, four correlation models can be adopted to correlate the solubility data. On the basis of the NRTL model, the dissolution thermodynamic properties, including enthalpy, entropy and Gibbs energy were calculated and discussed as well according to the experimental data, from which we conclude that the dissolution of 1-M-4-NP is an spontaneous process. Furthermore, solubility values and thermodynamic relations of 1-M-4-NP in selected solvents would be invoked as fundamental data and models regarding the purification process of 1-M-4-NP.

Keywords: Solubility; Correlation; Thermodynamic properties; 1-methyl-4-nitropyrazole