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Short Communication

Solubility and thermodynamics of terbinafine hydrochloride in different neat and binary solvents: Measurement, correlation and molecular interactions

Hongwei Shi, Yong Xie

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Highlights

- SLE of terbinafine hydrochloride in neat and binary solvent mixtures
- Values of the experimental solubility were correlated with different thermodynamic models.
- Thermodynamic properties of terbinafine hydrochloride dissolved in binary mixtures were evaluated.

Abstract

The solubility of terbinafine hydrochloride in four pure solvents, including methanol, ethanol, *n*-propanol and ethyl acetate and their binary solvent mixtures, including (methanol + ethyl acetate), (ethanol + ethyl acetate) and (*n*-propanol + ethyl acetate) performed at different mass fractions of methanol, ethanol or *n*-propanol ranging from 0.1 to 0.9, was determined by using isothermal saturation method with temperatures ranging from (278.15 to 313.15) K. The descending order of the mole fraction solubility in

pure solvents was as follow: methanol > ethanol > *n*-propanol > ethyl acetate, and for the three mixture with given initial composition, the solubility of terbinafine hydrochloride increased with increasing temperature and mass fraction of alcohol for the three systems including (methanol + ethyl acetate), (ethanol + ethyl acetate) and (*n*-propanol + ethyl acetate). At the same mass fraction of methanol, ethanol or *n*-propanol and temperature, the solubility of terbinafine hydrochloride was greater in (methanol + ethyl acetate) than in the other mixed solvents. The maximum mole fraction solubility of terbinafine hydrochloride was observed in methanol (6.297×10^{-2} at 313.15 K), followed by that in ethanol (3.785×10^{-2} at 313.15 K), *n*-propanol (3.007×10^{-2} at 313.15 K) and ethyl acetate (1.497×10^{-2} at 313.15 K)·The obtained solubility data were correlated with Jouyban-Acree model, van't Hoff-Jouyban-Acree model, modified Apelblat-Jouyban-Acree model and CNIBS/R-K model. The correlation showed good agreement with experimental results, the largest values of relative average deviations (*RAD*) and the root-mean-square deviations (*RMSD*) between the experimental and calculated solubility were 4.32×10^{-2} and 15.28×10^{-4}, respectively. On the basis of the obtained solubility, the standard enthalpy of solution (ΔH_{sol}^{o}), the standard Gibbs energy (ΔG_{sol}^{o}) of solution and the standard entropy of solution (ΔS_{sol}^{o}) of terbinafine hydrochloride dissolved in pure and mixed solvents were obtained by the famous van't Hoff calculations. Thermodynamic treatment of solubility data of terbinafine hydrochloride in these pure and mixed solvents by "Apparent thermodynamic analysis" indicated that the dissolution is an endothermic and entropy-driven process. The experimental solubility and the models in this study could be helpful in purifying the crude terbinafine hydrochloride.

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Keywords

Terbinafine hydrochloride; Solubility; Ethyl acetate; Modeling; Thermodynamic properties

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