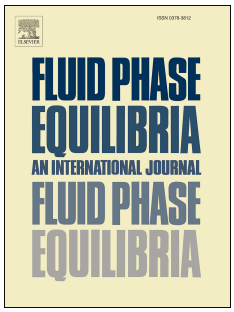

Solubility determination and correlation of cyromazine in sixteen pure solvents and mixing properties of solutions

Pengshuai Zhang, Rui Zhao, Chi Zhang, Tao Li, Baozeng Ren

PII: S0378-3812(18)30295-4

DOI: 10.1016/j.fluid.2018.07.024

Reference: FLUID 11901

To appear in: *Fluid Phase Equilibria*

Received Date: 24 April 2018

Revised Date: 22 July 2018

Accepted Date: 23 July 2018

Please cite this article as: P. Zhang, R. Zhao, C. Zhang, T. Li, B. Ren, Solubility determination and correlation of cyromazine in sixteen pure solvents and mixing properties of solutions, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.07.024.

Solubility determination and correlation of cyromazine in sixteen pure solvents and mixing properties of solutions

Pengshuai Zhang [a], Rui Zhao [a,b], Chi Zhang[a,c], Tao Li [a*], Baozeng Ren [a*]

a School of Chemical Engineering and Energy, Zhengzhou University, Zhengzhou 450001, PR China

b Henan chemical Technician College, Kaifeng, 475000, Henan, P. R. China

c Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Beijing 100080, PR China

Abstract:

The solubility of cyromazine in the pure solvents (methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, water, acetone, 2-propanol, isobutanol, 3-methyl-1-butanol and 2-butanol) at 283.15K to 323.15K, cyromazine in the pure solvents (acetic acid and acrylic acid) at 293.15K to 333.15K and cyromazine in the pure solvent of propanoic acid at 278.15K to 318.15K were measured by a laser dynamic method under atmospheric pressure. The experimental results show that the mole fraction solubility of cyromazine in the sixteen pure solvents decreased according to the following order: acrylic acid > acetic acid > propanoic acid > methanol > ethanol ≈ water > 1-propanol > 1-butanol >1-pentanol >1-hexanol > 1-heptanol > 3-methyl-1-butanol ≈ (2-propanol, 2-butanol, isobutanol and acetone). In order to facilitate industrial application (to improve the purity of cyromazine by crystallization in industry) and other research studies, the experimental solubility data are correlated with the five thermodynamic models: modified Apelblat equation, λh equation, non-random two liquid (NRTL) model equation, Wilson model equation and van't Hoff equation. Moreover, the mixing Gibbs energy ($\Delta_{mix}G$), mixing entropy ($\Delta_{mix}S$), mixing enthalpy ($\Delta_{mix}H$), activity coefficient (γ_1^{∞}) at infinitesimal concentration and reduced excess enthalpy ($H_1^{E,\infty}$) were obtained and the mixing process of cyromazine in the selected solvents are evaluated based on the Wilson model. The relatively close values of γ_1^{∞} and γ_1 indicated that the cyromazine -selected solvents solution systems are not highly non-ideal.

1. Introduction

Cyromazine (CAS Registry No. 66215-27-8) is one of the most commonly used biorational insecticide [1], its molecular formula is $C_6H_{10}N_6$ and the molecular structure is presented in Figure 1. The purity of the cyromazine depends on the crystallization processes, so it is essential to choose a proper solvent in the crystallization process. The solubility of cyromazine in the pure solvents (methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, water, acetic acid, propanoic acid, acrylic acid, 2-propanol, isobutanol, 3-methyl-1-butanol and 2-butanol) we selected have not been reported at present.

In this study, the solubility of cyromazine in the solvents at atmospheric pressure was measured by using a laser dynamic method. The experimental solubility data are correlated with the modified Apelblat equation, λh equation, non-random two liquid (NRTL) model equation, Wilson model equation and van't Hoff equation. Moreover, the mixing Gibbs energy ($\Delta_{mix}G$), mixing entropy ($\Delta_{mix}S$), mixing enthalpy ($\Delta_{mix}H$), activity coefficient (γ_1^{∞}) at infinitesimal

* Corresponding author. E-mail: renbz@zzu.edu.cn (Baozeng Ren). Tel: +86-371-67781267. Fax:+86-371-67781267; E-mail:litao912@zzu.edu.cn (Tao Li). Tel: +86-371-67781267. Fax:+86-371-67781267.