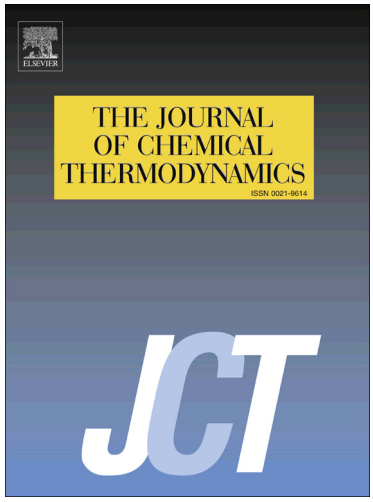
Accepted Manuscript



Construction and evaluation of ternary solid-liquid phase diagram of Pyraclostrobin (form IV) and its intermediate in ethanol and *N*,*N*-dimethylformamide

Cunbin Du, Ruimei Dong, Bin Qiao, Zhudan Jin, Tingting Ye, Ying Zhang, Mingliang Wang

PII: S0021-9614(18)30489-0
DOI: https://doi.org/10.1016/j.jct.2018.07.025
Reference: YJCHT 5482

To appear in: *J. Chem. Thermodynamics*

Received Date: 9 May 2018
Revised Date: 25 June 2018
Accepted Date: 28 July 2018

Please cite this article as: C. Du, R. Dong, B. Qiao, Z. Jin, T. Ye, Y. Zhang, M. Wang, Construction and evaluation of ternary solid-liquid phase diagram of Pyraclostrobin (form IV) and its intermediate in ethanol and *N*,*N*-dimethylformamide, *J. Chem. Thermodynamics* (2018), doi: https://doi.org/10.1016/j.jct.2018.07.025

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Construction and evaluation of ternary solid-liquid phase diagram of Pyraclostrobin (form IV) and its intermediate in ethanol and *N*,*N*-dimethylformamide

*Cunbin Du, Ruimei Dong, Bin Qiao, Zhudan Jin, Tingting Ye, Ying Zhang, Mingliang Wang**

School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, P. R. China.

Corresponding Authors: *Mingliang Wang* (wangmlchem@seu.edu.cn).

ABSTRACT

In order to improve the purity of target product and reduce the cost of industrial production, the phase diagrams of pyraclostrobin and its intermediate (pheny *N*-methoxy-*N*- (2- ((*N*'-pyrazinyl) pyrazolyl-3'-oxymethyl) -phenyl) carbamate) in binary and ternary systems was studied. In each ternary phase diagram, there were three crystallization regions (pure pyraclostrobin intermediate, pure pyraclostrobin, and mixture of pyraclostrobin and its intermediate), two co-saturated curves, and one co-saturated point. The crystallization region of pyraclostrobin intermediate was larger than that of pyraclostrobin in ethanol and *N*, *N*-dimethylformamide (DMF) at three temperatures. In order to extend application of the obtained binary and ternary systems, the NRTL model and Wilson model were used to describing the solubility behaviour of pyraclostrobin and its intermediate in binary and ternary systems, the value of root-mean-square deviation (*RMSD*) was no more 9.01×10^{-3}, the value of relative average deviation (*RAD*) was a little large, and no more than 5.84%. The calculated results via two models were all acceptable

Download English Version:

https://daneshyari.com/en/article/6659579

Download Persian Version:

https://daneshyari.com/article/6659579

Daneshyari.com