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Liquid-liquid equilibrium in binary systems of isomeric C₈ aliphatic monoethers with acetonitrile and its interpretation by the COSMO-SAC model

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Keywords

Liquid-liquid equilibrium; ether; acetonitrile; group contribution; UNIFAC, COSMO-SAC

Abstract

The liquid-liquid solubility curves have been determined by a synthetic method for six binary mixtures of acetonitrile + {heptyl methyl ether $- CH_3O^nC_7H_{15}$, or ethyl hexyl ether $- C_2H_5O^nC_6H_{13}$, or pentyl propyl ether ${}^nC_3H_7O^nC_5H_{11}$, or isopentyl propyl ether ${}^nC_3H_7O^iC_5H_{11}$, or dibutyl ether ${}^nC_4H_9O^nC_4H_9$, or butyl isobutyl ether ${}^nC_4H_9O^iC_4H_9$ }. The possibility of the COSMO-SAC model to account for the thermodynamic differences between these systems has been tested and the discussion on the influence of screening charge of ethers on the system properties was undertaken.

1. Introduction

The research on liquid-liquid equilibria is an important task for both applied and theoretical thermodynamics. Its practical significance refers to the extraction processes while adequate modelling still may be considered as a challenge, mainly because of strong temperature

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