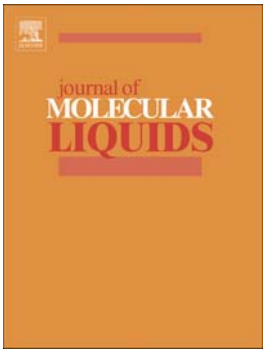

Phase behaviour of a continuous shouldered well model fluid. A grand canonical Monte Carlo study

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Phase behaviour of a continuous shouldered well model fluid. A grand canonical Monte Carlo study. *

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Abstract

The phase behavior of the continuous shouldered well model fluid proposed by Franzese [J. Mol. Liq. 136 (2007) 267] was examined using the Monte Carlo computer simulations in the grand canonical ensemble. The essential parts of the vapour-liquid and liquid-liquid coexistence envelopes were obtained. The Widom lines departing from coexistence envelopes were calculated using maxima of the fluctuations of the number of particles as a function of chemical potential along various isotherms. The region embracing anomalies in the properties of the model was located using the approximate criterion that involves the excess pair entropy.. The temperature of maximum density line was built by performing canonical Monte Carlo simulations. Our results are consistent with previous results from molecular dynamics constant pressure-constant temperature simulations and provide wider insight into the phase behavior of the model by using the chemical potential as the external parameter.

Keywords: liquids, soft-core model fluid, grand canonical Monte Carlo simulations, phase diagram

1. Introduction

Isotropic core-softened models of fluids have gained much of the scientific interest in two past decades. They can be considered as effective potentials and are the result of reducing some of the degrees of freedom of interaction between the molecules of the system. Since the form of the potential function is rather simple, i.e. containing no orientational inter-particle dependencies, these models are relatively easy to handle both computationally and theoretically. Despite the simplicity, it was shown that some of the core-softened models can still mimic complicated behaviour of anomalous real liquids, such as water [1], phosphorus [2], silica [3], triphenile phosphite [4], and others. In addition to

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