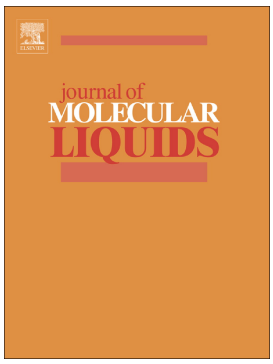

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Prediction of the critical properties of mixtures based on group contribution theory

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Abstract: A new simple model was proposed to predict the critical temperature (T_c) and critical pressure (p_c) of mixtures based on group contribution (GC) theory. In this model, the critical properties of mixtures can be predicted without critical parameters of each component. The experimental critical temperatures of 169 compounds and 379 binary mixtures as well as experimental critical pressures of 152 compounds and 188 binary mixtures were used to determine the group contribution parameters and model parameters. The average absolute relative deviations (AARDs) of correlation for compounds are 0.54% for T_c and 2.19% for p_c. AARDs of correlation for binary mixtures are 1.22% and 4.54% for T_c and p_c, respectively. The predictive ability of presented model was evaluated with T_c of 42 binary mixtures and 12 ternary mixtures as well as p_c of 8 binary mixtures and 12 ternary mixtures; predicted results agree well with experimental critical properties.

Keywords: critical temperature; critical pressure; group contribution; mixtures

1. Introduction

The critical properties including critical temperature, critical pressure, and critical volume are one of the most important thermophysical properties of fluids, which play a vital role in the description of phase behavior of mixtures, prediction of other physical parameters and development of equations of state [1, 2]. Additionally, they are essential parameters in many