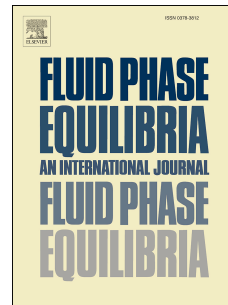


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Enthalpy of Vaporization, Its Temperature Dependence And Correlation With Surface Tension: A Theoretical Approach

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Abstract:

Enthalpy of vaporization is one of the most important thermophysical properties due to its extensive applications in science and industry. Prediction of the enthalpy of vaporization as a function of temperature has been the topic of many studies in the past decades. Among numerous models available in the literature, only a few of them which are empirically developed provide accurate results for all compounds and no theoretical approach has led to a successful model to date. In the present study, exploiting the statistical and classical thermodynamics of the evaporation and condensation and with some simplifying assumptions, an expression was developed on a fully theoretical basis to predict the vaporization enthalpy of pure compounds at various temperatures. The predictability of the new model was evaluated for 1890 compounds for a temperature range from 50 K below the normal boiling point to 100 K below the critical temperature and resulted an average absolute relative error of 4.49 % and an average correlation coefficient of 0.9959 which are comparable with the results of the most accurate empirical models. The veracity of the approach was verified through investigating the significance of the terms appearing in the proposed expression as well as the influence of the simplifying assumption on the accuracy of results. Through the proposed approach, a widely applied empirical correlation between the enthalpy of vaporization and surface tension was theoretically derived.

Keywords: enthalpy of vaporization, surface tension, evaporation, condensation, transition state theory

1- Introduction

Enthalpy of vaporization is one of the most important thermophysical properties of substances due to its extensive applications in science and industry. Molar enthalpy of vaporization is defined as the enthalpy change for transferring one mole of evaporating molecules from liquid to gas phase.

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