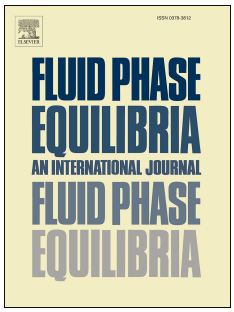
Accepted Manuscript



Estimation of the enthalpy of vaporization at normal boiling temperature of organic compounds by a new group contribution method

Soheil Abdi, Kamyar Movagharnejad, Habib Ghasemitabar

PII: S0378-3812(18)30242-5

DOI: 10.1016/j.fluid.2018.06.006

Reference: FLUID 11861

To appear in: *Fluid Phase Equilibria*

Received Date: 15 March 2018

Revised Date: 13 June 2018

Accepted Date: 14 June 2018

Please cite this article as: S. Abdi, K. Movagharnejad, H. Ghasemitabar, Estimation of the enthalpy of vaporization at normal boiling temperature of organic compounds by a new group contribution method, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.06.006.

Estimation of the enthalpy of vaporization at normal boiling temperature of organic compounds by a new group contribution method

Soheil Abdi, Kamyar Movagharnejad*, Habib Ghasemitabar

Babol Noshiravani University of Technology, Faculty of Chemical Engineering, Babol, Iran

Abstract

We need to know the thermo-physical properties of different compounds in order to design, model or optimize the industrial processes. Among various thermo-physical properties, enthalpy of vaporization at normal boiling temperature is one of the most important and useful properties in industrial processes. Although experimental data are available from various sources, but in order to complete these data, theoretical methods may be required to estimate and predict this property. The new group contribution method which can be regarded as a modification to the original Joback and Reid method gives more accurate estimations of the enthalpy of vaporization at normal boiling temperature of organic compounds. Group contribution values have been optimized using 3950 experimental data of organic components with a molecular weight range of 28-565($g.mol^{-1}$) and number of carbon atoms range of 1-40. Checking the results of the new method on 3950 different organic compounds shows an average absolute error of 0.620 kJ/mol and the percentage average relative error of 1.683%. The results of the new method have been compared with the original method of Joback and Reid, and the Kolska, Ruzicka and Gani method. The results showed the better agreement between the predictions of the present method and the experimental data, comparing to the other group contribution methods.

Key words: enthalpy of vaporization; normal boiling temperature; group contribution method; organic compounds

Introduction

A good knowledge about the thermo-physical properties is essential for every engineering design and calculation. For example, an engineer would not be able to design a bridge without having detailed information about the properties of concrete or steel. Similarly, a good knowledge of thermodynamic properties are required for any chemical engineer in order to design a variety of products, processes or industrial equipment [1]. Experimental methods and laboratory measurements of thermo-physical properties require a lot of time and money

* Corresponding author Email: movagharnejad@yahoo.com