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High-pressure liquid densities of fatty acid methyl esters:

Measurement and prediction with PC-SAFT equation of state

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ABSTRACT

In this work, experimental density data were reported for six fatty acid methyl esters,

including methyl butyrate, methyl valerate, methyl caproate, methyl pelargonate, methyl

heptanoate, and methyl caprylate. The densities were measured from 293.15 K to 363.15 K and

pressures up to 60 MPa by a vibrating-tube densimeter. The relative uncertainty of the

measurement is estimated less than 0.001 with a confidence level of 0.95. The high pressure

densities were correlated with a Tait-type equation. The overall average relative deviation between

experimental data and calculated results from Tait equation for the six fatty acid esters is 0.010 %.

The derived thermodynamic properties, such as isobaric thermal expansivity and isothermal

compressibility, were obtained from the experimental density results. Additionally, for the studied

esters, the molecular parameters of the PC-SAFT equation of state were obtained based on the

corresponding vapor pressures and liquid densities. The PC-SAFT equation was used to predict

the high pressure densities of the esters, and good agreements were observed.

Keywords: Fatty acid methyl esters; High-pressure liquid density; Derivative properties;

PC-SAFT equation

Introduction

Fatty acid esters, including fatty acid methyl esters (FAMEs) and fatty acid ethyl esters

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