Stereoisomeric Effects on Volumetric Properties under Pressure for the System Cis- + Trans-Decalin

Y. Miyake, A. Baylaucq[C, S], C.K. Zeberg-Mikkelsen and C. Boned
Laboratoire des Fluides Complexes, Faculte des Sciences et Techniques, Universite de Pau, Pau, France
antoine.baylaucq@univ-pau.fr

G. Galliero
Laboratoire d'Etude des Transferts d'Energie et de Matiere, Universite de Marne-la-Vallee, Marne la Vallee, France

H. Ushiki
Department of Environmental and Natural Resource Science, Tokyo University of Agriculture and Technology, Fuchu-shi, Tokyo, Japan

In order to study the influence of the stereoisomeric effects on the volumetric properties, an extensive experimental study of the density of the asymmetrical binary system cis-trans-decalin has been performed (294 points) for 7 different compositions including the pure compounds at three temperatures, 303.15, 323.15 and 343.15 K and fourteen isobars up to 65 MPa with a vibrating-tube densimeter; the experimental relative uncertainty is estimated to be 0.05 %. The isothermal compressibility, the isobaric thermal expansivity, and the excess molar volume have been derived. The results have been interpreted as changes in the molecular free-volume, disruption of the order molecular structure, and the breaking or formation of molecular interactions. In order to evaluate the performance of different analytical equations of state (EOS) to take into account stereoisomeric effects, the PC-SAFT EOS using one adjustable binary interaction parameter and the PR EOS with the modified Huron-Vidal mixing rule and the UNIFAC model are applied on the binary system cis-trans-decalin. In addition molecular dynamic simulations using the Lennard Jones representation is also discussed.