

Nitta Chao model prediction for the binary diethyl carbonate + n-decane

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This work present the study of the experimental high-pressure density data for diethyl carbonate + n-decane binary system, in the range of pressures between 0.1 MPa to 40 MPa, and in the range of temperatures from 288.15 K to 308.15 K. The experimental values were predicted by Nitta –Chao group contribution model.

This system of diethyl carbonate + n-decane have been considered as replacement of traditional oxygenated gasoline additive, because is non-toxic and environmentally friendly products capable to reduce pollutant emissions as carbon monoxide.

Nitta-Chao is a model for the prediction of density, is based on the group contribution model, with the repulsive forces between molecules. This model have advantages for his theoretical rigor. Diethyl carbonate and n-decane were described by the molecular groups, methyl (-CH₃), methylene(-CH₂) and carbonate (-OCOO-)

Present work reports valuable experimental high-pressure density for the binary mixture diethyl carbonate + n-decane in the range of temperature from 288.15 to 308.15 and pressures from 0.1 MPa to 40 MPa.

The values of high pressure density were determinated for all the range of molar fraction of the system. Figure 1 shows the example of the experimental data obtained for $x_1=0.5032$ for the high pressure density. The interactions between aliphatic groups and polar groups are dispersive.

Nitta Chao is a model who predict correctly the high pressure density for this systems.

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