

Volumetric properties modeling of binary mixtures by Prigogine-Flory-Patterson (PFP) and Extended Real Association Solution (ERAS) models

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In this work, excess molar volume, V^E , of two previously published binary systems, dimethyl adipate+1-butanol and dimethyl adipate+2-butanol were correlated with two models, Prigogine-Flory-Patterson (PFP) and Extended Real Association Solution (ERAS).

Volumetric coefficients, thermal expansion coefficient, α , and isothermal compressibility, κ , were calculated from density, speed of sound and isobaric heat capacity data. Isobaric molar heat capacities, C_p , at all temperatures for 2-butanol were obtained by correlation of literature data using Jovanović et al. model, while heat capacities for dimethyl adipate were predicted with Kolskà *et al.* model.

PFP and ERAS models were used for analysis of molecular interactions present in the investigated solutions.

Modelovanje volumetrijske osobina binarnih smeša korišćenjem Prigogine-Flory-Patterson (PFP) i Extended Real Association Solution (ERAS) modela

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U ovom radu, dopunske molarne zapremine, V^E , dva prethodno objavljena binarna sistema, dimetil adipat+1-butanol i dimetil adipat+2-butanol korelisane su sa dva modela, Prigogine-Flory-Patterson (PFP) i Extended Real Association Solution (ERAS) modelom.

Volumetrijski koeficijenti, koeficijent termalne ekspanzije, α , i izotermalne kompresibilnosti, κ , izračunati su preko podataka za gustinu, brzine zvuka i izobarske toplotne kapacitivnosti. Izobarski molarni toplotni kapaciteti, C_p , na svim temperaturama za 2-butanol dobijeni su koreljanjem literaturnih podataka koristeći Jovanović *et al.* model, dok su toplotni kapaciteti za dimetil adipat dobijeni preko Kolskà et al. modela.

PFP i ERAS modeli primenjeni su za analizu molekulskih interakcija prisutnih u datim smešama.