New Group Interaction Parameters of the UNIFAC model: Aromatic carboxylic acid isomers Binaries.

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Abstract

With the available solid-liquid equilibrium (SLE) data of six aromatic carboxylic acids (aromatic dicarboxylic acid isomers (terephthalic acid (TPA), isophthalic acid (IPA), phthalic acid (PA)) and methyl benzoic acid isomers (m-toluic acid (m-TA), o-toluic acid (o-TA), p-TA)) in HOAc + H2O solvent mixtures, the relationship between the molecular structure of above aromatic carboxylic acids and the solubility of them in HOAc + H2O solvent mixtures is discussed. Meanwhile, three new groups p-ArCOOH, m-ArCOOH and o-ArCOOH in UNIFAC (Dortmund) model were firstly defined to distinguish the influence of the positions of ArCOOH on thermodynamic properties of aromatic carboxylic acid isomers, which indicate the ArCOOH located in para, meta and ortho positions of the ArCOOH or ArCH3 groups respectively. Then the interaction parameters of the ArCOOH, p-ArCOOH, m-ArCOOH and o-ArCOOH with other involved groups in the solvent systems are firstly obtained by regressing these available SLE data.

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