Application of simplified PC-SAFT to glycol ethers

The simplified PC-SAFT (sPC-SAFT) equation of state is applied for binary glycol ether-containing mixtures, and it is investigated how the results are influenced by inclusion of intramolecular association in the association theory. Three different glycol ethers are examined: 2-methoxyethanol, 2-ethoxyethanol, and 2-butoxyethanol. Vapor-liquid and liquid-liquid equilibria of miscible and immiscible, self- and cross-associating mixtures are considered, including the closed-loop liquid-liquid equilibrium of 2-butoxyethanol-water. The results are finally compared to other association models. © 2011 American Chemical Society.

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