The 'State Conditions Transferability' category of IFPSC 2006 tests prediction of binary vapor–liquid isotherms for mixtures of ethanol and the refrigerant HFF-227ea (1,1,1,2,3,3,3-heptafluoropropane). We predict these isotherms using fluctuation solution theory (FST). The method is based on isobaric–isothermal molecular dynamics (NPT-MD) simulations, using force field parameters published in the literature and fitted CHARMM force field parameters. Systems studied previously [S. Christensen, G.H. Peters, F.Y. Hansen, J.P. O’Connell, J. Abildskov. Molecular Simulation 33 (2007) 449–457] comprise the nearly ideal benzene/methyl acetate system, and the less ideal benzene/ethanol system at ambient temperatures. Both are at low pressures and remote from the pure component critical points. For the IFPSC system, we have used the same method even though predictions are for conditions remote from those of the provided data, the pressures are elevated, and the temperatures are near the critical temperature of one of the components. We first describe the computational method and thermodynamic modeling for the entry submitted, which assumed the vapor was an ideal gas and no Poynting correction was included. Then we discuss the effects of using common modeling methods to estimate the effects of elevated pressures.

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