The Critical Solution Behavior of C5-diol isomers in Carbon Dioxide

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We determined the phase behavior of the binary mixtures of (2,2-dimethyl-1,3-propanediol + CO_2) and (2,4-pentanediol + CO_2). 2,2-dimethyl-1,3-propanediol and 2,4-pentanediol are C5-diols isomers. 2,2-dimethyl-1,3-propanediol has two hydroxyl groups that are located at the opposite end sites of its structure. 2,2-dimethyl-1,3-propanediol also has two methyl groups connected to the center carbon, which makes its molecular structure cross-like. The unique molecular structure of 2,2-dimethyl-1,3-propanediol influences the degree of intra- and inter-molecular hydrogen bonding of the diol. 2,4-pentanediol has two hydroxyl groups at the second and the fourth carbon in the straight carbon structure, so it is expected that the degree of intramolecular hydrogen bonding of 2,4-pentanediol is higher than that of 2,2-dimethyl-1,3-propanediol. The experimental P-T diagrams and P-x isotherms of the two diols in CO_2 were simulated with Peng-Robinson EOS. The pure component parameters, such as critical temperature and pressure, boiling temperature, and acentric factor, of the two diols were calculated using Marrero and Gani group contribution model and Amborse and Walton suggestion. Whereas the P-x isotherms modeled with PR EOS.