The Effect of Molecular Structure of C_5-diols on the Phase Behavior of C_5-diols + Carbon Dioxide Mixture

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We determined the phase behavior of the binary mixtures of 2,2-dimethyl 1,3-propanediol (NPG) + CO2 and 2,4-pentanediol (2,4-PDOH) + CO2. NPG and 2,4-PDOH are C5-diol isomers that have two hydroxyl groups and five carbons. The phase transition pressures, from homogenous phases to dew- or bubble-point, of (NPG + CO2) mixture is much higher than the transition pressures of (2,4-PDOH + CO2). The difference in the phase transition pressure is the consequence of the different positions of two hydroxyl groups in the C5-diols. NPG has two hydroxyl groups at the 1 and 3 carbons and two methyl groups at the middle carbon. The two hydroxyl groups of NPG are separated by the end carbons and the carbon whose two hydrogens are substituted with methyl groups. NPG is not expected to perform intramolecular hydrogen bonding due to its unique molecular structure, which affect the degree of intermolecular attraction between NPG molecules. 2,4-PDOH has linear structure and the two hydroxyl groups locate at 2 and 4 carbons. The degree of intramolecular hydrogen bonding of 2,4-PDOH is expected stronger than that of NPG, which reduces the intermolecular attraction between 2,4-PDOH molecules. The P-x isotherms of the two diols in CO2 were correlated with P-R EOS.