Experimental solubility data of two solid derivatives of menadione in supercritical carbon dioxide: 2-((4-chlorobenzyl)amino)-3-methylnaphtalene-1,4-dione, and 2-((4-chlorophenethyl)amino)-3-methylnaphtalene-1,4-dione

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Abstract

Two solid derivatives of vitamin K3 or menadione, 2-((4-chlorobenzyl)amino)-3-methylnaphthalene-1,4-dione and 2-((4-chlorophenethyl)amino)-3-methylnaphthalene-1,4-dione, were synthesized and chemically characterized with a purity of 98 % mol·mol−1. The solubility (molar fraction) of each derivative in high-pressure carbon dioxide was measured using an analytic-recirculation methodology at (313, 323 and 333) K, and pressures from (8.72–33.67) MPa. The solubility values were from (22·10-6 to 99·10-6) mol·mol−1, and from (48·10-6 to 223·10-6) for 2-((4-chlorobenzyl)amino)-3-methylnaphthalene-1,4-dione and 2-((4-chlorophenethyl)amino)-3-methylnaphthalene-1,4-dione respectively. Questionable experimental data points were detected calculating the combined expanded uncertainty, applying the thermodynamic consistency and the self-consistency tests, as well as analyzing the chemical structure of the solute after it had been measured. The solvent power of the high-pressure carbon dioxide over the synthesized menadione solid derivatives was studied based on the parameters of the equation of Chrastil adjusted to the experimental data, in order to have evidence of the relationship between solute molecular structure and solubility.