

Solibilities of Caffeine, Theophylline and Theobromine in Water and the Density of Caffeine Solutions

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ABSTRACT

Caffeine, theophylline and theobromine are important ingredients of coffee, tea, maté, guarana and cacao, respectively. Although very similar in molecular constitution, they differ nevertheless, widely in many physical properties. The solubility of the three compounds, for instance, is very different. The solubility of these pureness in water has been measured over a wide temperature range using different experimental techniques. The effect of pH on solubility and crystallisation behaviour has also been studied. The exact knowledge of these properties is important for extraction processes of the purines (e.g. recovery from CO₂ decaffeination process solutions, water decaffeination) or from waste materials as well as for separation and purification techniques or pharmaceutical applications. Furthermore, the density of aqueous caffeine solution along the saturation line has been determined with precision. This enables continuous concentration measurement of process solutions by an in-flow density meter.