Vapor–Liquid Equilibria Measurements of Bitter Orange Aroma Compounds Highly Diluted in Boiling Hydro-Alcoholic Solutions at 101.3 kPa

Sophie Deterre, † Joe "1 Albet, \ddagger , § Xavier Joulia, $\#, \bot$ Olivier Baudouin, \triangledown Pierre Giampaoli, † Martine Decloux, † and Violaine Athe s*,#

† AgroParisTech, INRA, and Cnam, UMR1145 Ingénierie Procédés Aliments, 1 av. des Olympiades, F-91300 Massy, France

‡ INRA, UMR 1010, ENSIACET, 4 allée Emile Monso, F-31030, Toulouse Cedex 4, France

§ Université de Toulouse, INPT, UMR 1010, 4, Allée Emile Monso, F-31030 Toulouse, France

Université de Toulouse, INPT, UPS, Laboratoire de Génie Chimique, 4, Allée Emile Monso, F-31030 Toulouse, France

CNRS, Laboratoire de G**é**nie Chimique, F-31030 Toulouse, France

ProSim SA, Stratège Bât. A, 51, rue Ampère, BP 27210, F-31672 Labège Cedex, France

Unité Mixte de Recherche UMR782 Génie et Microbiologie des Procédés Alimentaires, AgroParisTech/INRA, Avenue Lucien Brétignières, F-78850 Thiverval-Grignon, France

ABSTRACT:

In this work, experimental vapor–liquid equilibria (VLE) of water + ethanol + five aroma compound (two monoterpene hydrocarbons, α -pinene and D-limonene, and three oxygenated compounds, linalool, citral, and linalool oxide) mixtures were measured at boiling point at 101.3 kPa for ethanol molar fractions ranging from 0.0140 to 0.8389. The five aroma compounds were selected for their strong contribution to the aroma of the distillate of bitter orange essential oil. First, the thermodynamic consistency of the experimental VLE data was validated. Then the NRTL and Henry's law type models were tested to correlate the experimental data. Good agreement was obtained with both models to predict the phase equilibrium of the oxygenated compounds, and a better

J. Chem. Eng. Data, 2012, 57 (12), pp 3344–3356 **DOI:** 10.1021/je3004854 Publication Date (Web): November 14, 2012 Copyright © 2012 American Chemical Society