

Vapor Pressures of Oxygenated Compounds using a Step Potential Perturbation Method

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Experimental measurements of thermodynamic properties of bio-derived chemicals are scarcer than properties for hydrocarbons of similar molecular weight and therefore reliable predictive methods are desirable. For example, vapor pressures of ethyl esters of fatty acids are scarce. Other bioderived compounds are difficult to purify. For example, acetylation of glycerol simultaneously produces two isomers of 4-hydroxymethyl-2-methyl-1,3-dioxolane and two isomers of 5-hydroxy-2-methyl-1,3-dioxane, all with similar boiling points. In this work, we extend the SPEAD method (Baskaya, F. S.; Gray, N. H.; et al., *Fluid Phase Equil.* 2005, 236, 42-52) to heavy esters, secondary alcohols, cyclic hydrocarbons and cyclic ethers, and multifunctional compounds such as the cyclic acetals and ethyl lactate. We present the transferrable group parameters and discuss capabilities and considerations for vapor pressure predictions.