

An Equation for the Correlation of Water + n-Alkane Binary Systems Interfacial Tension Data and Prediction of this Quantity for Binaries of Water + Branched Isomers of Alkanes

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This work presents an equation for the correlation of interfacial tension data of binary systems formed by water + n-alkanes. The equation uses the molecular mass as the property that rationalizes the behavior of interfacial tension for systems having a common component (water) and components from a homologous series like n-alkanes; the functionality with temperature is also considered in this correlation using an inverse reduced temperature scale, in a similar way as used in previous work from the authors, where this equation was used to represent the surface tension of pure hydrocarbons¹. To test the proposed equation, we have carried out the correlation of 94 experimental interfacial tension values from the literature for systems water + n-alkanes (n-hexane to n-dodecane) covering the temperature range 303 to 343 K, with a standard deviation of 0.12 mN·m⁻¹. Also, a new scheme for the prediction of interfacial tension values for binary systems water + isomer of n-alkanes which uses the isomerism surface tension parameter (IST) reported in a previous work from the authors² is presented. This prediction scheme takes advantage of the correlation mentioned above to derive the interfacial tension value for a given water + n-alkane system, which in turn is modified by the IST parameter to obtain that corresponding to water + isomer of n-alkane system. This procedure can also be used to predict interfacial tension values at different temperatures, at least in the interval covered by the correlation. The prediction scheme was tested with 5 binaries: water + n-alkane isomer (2-methylpentane, 3-methylpentane, 2,3-dimethylpentane, 2,2,4-trimethylpentane, and 2,3,4-trimethylpentane) using 21 experimental points at different temperatures between 303 and 343 K, obtaining an average relative error of 3.48 %.

[1] Romero-Martínez, A.; Trejo, A. *Int. J. Thermophys.* 19, 1998. 1605-1614.

[2] Romero-Martínez, A.; Trejo, A.; Murrieta-Guevara, F. *Fluid Phase Equilib.* 171, 2000, 1-10.