Universal scaling behaviour of surface tension of molecular chains

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We use and extend the universal relationship recently proposed by Galliero,[1] based on a combination of the corresponding-states principle of Guggenheim[2] and the parachor approach of Macleod[3], to predict the vapour-liquid surface tension of fully flexible chainlike Lennard-Jones molecules. In the original study of Galliero, the reduced surface tension of short-chain molecules formed by up to five monomers is expressed as a unique function of the difference between the liquid and vapour coexistence densities.

In this work, we extend the applicability of the recipe and demonstrate that it is also valid for predicting the surface tension of two different chainlike molecular models, namely, linear tangent chains that interact through the Lennard-Jones intermolecular potential and fully flexible chains formed by spherical segments interacting through the square-well potential. Computer simulation data for vapour-liquid surface tension of fully flexible and rigid linear Lennard-Jones, and fluid flexible square-well chains is taken from our previous works. Our results indicate that the universal scaling relationship is able to correlate short- and long-chain molecules with different degrees of flexibility and interacting through different intermolecular potentials.

G. Galliero, J. Chem. Phys. 133, 074705 (2010) E. A. Guggenheim, J. Chem. Phys. 13, 253 (1945) J. Macleod, Trans. Faraday Soc. 19, 38 (1923)

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