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Thermodynamic Properties of Alcohols Using Molecular Dynamics Simulations.[1] ABDALLA OBEIDAT, HIND ABU GHAZLEH, Jordan University of Science and Technology — Thermodynamic properties of methanol, ethanol and propanol such as: density, surface tension and dipole moment have been estimated as a function of temperature using two different potential functions (OPLS-AA and TraPPE-UA). Our results have been compared to experimental values at low temperatures; from 200K to 300K. The results are quite satisfactory, and one cannot judge the best potential function in studying these unary systems.

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Abdalla Obeidat
Jordan University of Science and Technology

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