

Prediction of Minimum Flash Point Behavior for Binary Mixtures

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ABSTRACT

Flash point is a primary property used to determine the fire and explosion hazards of a liquid. Minimum flash point behaviour (MFPB) is exhibited when the flash point of a mixture is below the flash points of the individual components. The identification of this behaviour is critical, because a hazardous situation results from taking the lowest component flash point value as the mixture flash point. Even for experimental measurements, an estimate of the mixture flash point is needed. A procedure to estimate the flash point of binary mixtures is discussed. Predictions for the aqueous mixtures methanol–water and ethanol–water are presented and compared with experimental values as well as for the flammable mixtures octane–ethanol and octane-1-butanol, which exhibit MFPB. Quantum chemical calculation methods such as COSMO-RS and theoretical methods such as UNIFAC were evaluated for the prediction of MFPB mixtures.