

Predictive Methods: Are Experimental Measurements Still Necessary

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Knowledge of thermochemical and thermophysical properties is required in the design and optimization of many chemical engineering and pharmaceutical processes. The required experimental values are often not readily available, and researchers have turned to predictive methods as a means to generate thermochemical and thermophysical properties needed as input values in design calculations. Discussion will focus on the thermodynamic properties associated with the different phase transitions. The larger databases containing experimental thermodynamic phase transition data will be discussed, and methods given for determining whether or not the published experimental values are internally consistent. The different predictive methods for calculating enthalpies and entropies of fusion, vaporization and sublimation will be reviewed, and examples will be given to illustrate each computational method. Calculated values will be compared to available data to assess the applications and limitations of each predictive method. Such comparisons provide an indication of whether existing predictive methods have now reached the point to where experimental measurements are no longer necessary. In addition, examples will be given of where predictive methods have been used to screen experimental data and to identify incorrect experimental values in need of redetermination.