Rapid Evaluation of Prediction Methods with DIPPR's Automated Property Prediction Package

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An automated property prediction package has been developed, that permits rapid evaluation of group-contribution, corresponding states, empirical, and theoretical property estimation methods. The property prediction package, which is part of the DIPPR® Information And Data Evaluation Manager (DIADEM) software, is used in conjunction with the DIPPR® 801 database, to develop and test new prediction methods. The estimation engine is based on an automated SMILES formula parser, to provide required molecular structural information, retrieval of required secondary properties from the DIPPR® database, and defined rules for the method. Automated comparisons of predicted values to experimental data in the DIPPR® database can be made for properties at specified accuracy levels, by the chemical family or type, or over the entire database. This allows for an evaluation of the relative effectiveness of methods for specific chemical families, and a tailoring of the selected method to specific chemical classes. New methods can readily be added by input to a simple rule table, a group value table (as required), and a priority definition table. Over 100 thermophysical property prediction methods are currently available in DIADEM. The evaluation of several methods for critical point estimation will be discussed in order to illustrate the use of this method to evaluate prediction methods.