

The DIPPR® 801 Database/DIADEM Software: Evaluated, Dynamic, and Simulator-Ready

Nathan Lott^{C,S}

DIPPR, New York, NY, U.S.A.

dippr@aiche.org

Thomas Knotts

Chemical Engineering Department, BYU, Provo, UT, U.S.A.

The DIPPR® 801 Database is a collection of thermo-physical property data with an emphasis on quality through a rigorous “systems-approach” evaluation procedure, currency by continually improving existing and adding new content, and completeness to ensure simulator-readiness.

Evaluated: DIPPR® 801 uses a systems approach in evaluating all available data for a given compound to triangulate on the best values and produce higher accuracy than could be achieved using only individual points. This approach includes hundreds of applied constraints such as inter-property relationships, expected smooth trends of properties between related chemicals, and the impact of chemical similarities and differences. Once these constraints are simultaneously satisfied for all properties, experts manually review and give final approval. Therefore, each compound in the database has evaluated, expert-recommended values for all properties.

Dynamic: New compounds and properties are added to the database each year, while improvements are made to data and correlations of existing compounds as new experimental data and prediction methods are discovered through an extensive frequent world-wide search of published and sponsor-donated data.

Simultor-Ready: DIPPR® 801’s vast collection of evaluated data is used to test and refine prediction methods such that when experimental data are not available, values for properties are predicted using prediction methods proven accurate for similar compounds. These predicted values are also subject to the same rigorous systems-level evaluation process mentioned previously. This eliminates “holes” such that accurate results are almost always achievable in simulation software packages.

The DIPPR® Interface and Data Evaluation Manager (DIADEM) is an interface and data analysis tool designed for use with the DIPPR® 801 database and with user-developed databases. Among other powerful features, DIADEM contains a 200-method property prediction package that enables users to obtain accurate estimated property values for any compound whether or not it is included in the DIPPR® 801 Database.