

Proper Use of the DIPPR 801 Database for Creation of Models, Methods, and Processes

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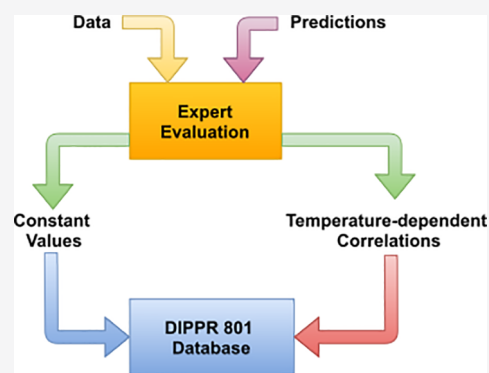
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ABSTRACT: The Design Institute for Physical Properties (DIPPR) maintains the DIPPR 801 database for the American Institute of Chemical Engineers. The 801 database is the largest collection of critically evaluated, pure-species, thermophysical property data in the world and is used by engineers and academics. This paper is a response to misuse of the DIPPR 801 database in the literature. To help researchers avoid misuse, the critical evaluation process for property values is explained, and common mistakes that occur in the literature are outlined. A guide to using the DIPPR database for both academic and industrial use is also included.



INTRODUCTION

In 1980, the American Institute of Chemical Engineers (AIChE) established the Design Institute for Physical Properties (DIPPR), a research consortium supported by member companies, to respond to various industrial needs for reliable and consistent thermophysical property data. Currently, DIPPR maintains and expands the DIPPR 801 Database which is the “Gold Standard” for pure-component property values. The DIPPR 801 database is located at Brigham Young University in Provo, Utah and derives its name from Provo’s area code. This database is characterized by two hallmarks: accuracy and completeness. “Complete” means that every compound in the database contains recommended values for all properties, a feat accomplished by using state-of-the-art prediction methods to obtain property values when no reliable experimental data are available. Because of the accuracy and completeness provided by the DIPPR 801 database, many groups use the database to do fundamental research. Unfortunately, many investigators have done so without a proper understanding of the database, which has led to dubious scientific claims.

This article is a response to instances where authors have misused DIPPR 801 database content. This commonly arises from the misinterpretation of the database. All physical property values in the database must be understood in the context of DIPPR’s evaluation process to be used correctly. Therefore, this work aims to promote a better understanding of the evaluation process and definitions used in the DIPPR 801 database, leading to appropriate use of database values.

This work will begin with an overview of the DIPPR 801 database to provide the background needed to understand the proper use of the database. The role of the DIPPR 801 Project in providing high quality chemical profiles will be covered as well as common mistakes made while using the database and how to avoid them. Finally, the best practices for use of the DIPPR database in scientific literature and research will be explained.

Explanation of DIPPR Evaluation Processes. Many mistakes made using DIPPR values can be avoided by a better understanding of the DIPPR database and the evaluation processes used in its development. DIPPR’s evaluation process is what makes the DIPPR database the Gold Standard for thermophysical data. Relevant details of the database and the evaluation process are discussed below.

Overview. The goal of the DIPPR 801 database is to provide the most accurate and complete thermophysical property data for the 32 constant and 15 temperature-dependent properties in the database for pure compounds of industrial importance, listed in [Tables 1 and 2](#). This focus on industrial needs means it is not the largest database in terms of number of compounds, nor are all possible thermophysical properties found in the database. Rather, both the compounds

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Table 1. Available Pure-Component Constant Physical Properties Studied and Recommended in the DIPPR 801 Database^a

constant properties	constant properties (cont.)
Molecular Weight (MW)	Standard Absolute Entropy (SSTD)
Critical Temperature (TC)	Heat of Fusion at Melting Point (HFUS)
Critical Pressure (PC)	Standard Net Heat of Combustion (HCOM)
Critical Volume (VC)	Flash Point (FP)
Critical Compressibility Factor (ZC)	Lower Flammability Limit Composition and Temperature (FLVL/FLTL)
Acentric Factor (ACEN)	Upper Flammability Limit Composition and Temperature (FLVU/FLTU)
Normal Boiling Point (NBP)	Autoignition Temperature (AIT)
Melting Point (MP)	Radius of Gyration (RG)
Triple Point Temperature (TPT)	Solubility Parameter (SOLP)
Triple Point Pressure (TPP)	Dipole Moment (DM)
Liquid Molar Volume (LVOL)	van der Waals Volume (VDWV)
Ideal Gas Enthalpy of Formation (HFOR)	van der Waals Area (VDWA)
Ideal Gas Gibbs Energy of Formation (GFOR)	Refractive Index (RI)
Ideal Gas Absolute Entropy (ENT)	Heat of Sublimation (HSUB)
Standard Heat of Formation (HSTD)	Parachor (PAR)
Standard Gibbs Energy of Formation (GSTD)	Dielectric Constant (DC)

^aAbbreviations used by DIPPR are given in parentheses.

Table 2. Available Pure-Component Temperature-Dependent Physical Properties Studied and Recommended in the DIPPR 801 Database^a

Temperature-Dependent Properties	Temperature-Dependent Properties (cont.)
Solid Density (SDN)	Thermal Conductivity of Liquid (LTC)
Liquid Density (LDN)	Thermal Conductivity of Solid (STC)
Heat Capacity of Ideal Gas (ICP)	Thermal Conductivity of Vapor (VTC)
Heat Capacity of Liquid (LCP)	Vapor Pressure of Liquid (VP)
Heat Capacity of Solid (SCP)	Vapor Pressure of Solid or Sublimation Pressure (SVP)
Heat of Vaporization (HVP)	Viscosity of Liquid (LVS)
Second Virial Coefficient (SVR)	Viscosity of Vapor (VVS) Surface Tension (ST)

^aAbbreviations used by DIPPR are given in parentheses.

and associated properties in the database are carefully curated so that users can be confident that needed data are both available and accurate.

The quality of the database depends on a well-developed evaluation process. Broadly, the process includes:

1. A survey of all the available data for the compound found in the literature
2. An assessment of the quality of the data
3. Predictions of property values when no experimental data exist
4. Testing all data and predictions against rigorous thermodynamic relationships and empirical heuristics
5. Assignment of uncertainties to values
6. Expert evaluation of the selections by at least three experts from academia and industry

This process is intended to involve evaluations of data by several individuals. This human element in the process allows careful alterations to achieve a result that is complete, consistent with literature, and self-consistent. The evaluation process is iterative as correlation models, methods, and best data sources are updated until a Gold Standard chemical profile is built that represents the best information related to the physical properties. Such thorough evaluation is needed because sponsors and other database users employ DIPPR recommended values for process design, simulation, and research purposes. The following sections discuss unique elements of the evaluation process and how they contribute to the quality and utility of the database.

Some words should be defined in this context before our discussion:

- **Data:** information based on an experimental result
- **Value:** a database entry that can include experimental and/or predicted information
- **Correlation:** a temperature-dependent equation for a property that has been fitted with experimental and/or predicted values
- **Accepted value or correlation:** a value or correlation recommended by DIPPR in the 801 Database because it has been found to be the most reliable and consistent information available
- **Predicted value:** a database entry that was produced from any kind of prediction or estimation method; used interchangeably with estimated value

Industrial Sponsorship. More than 40 companies and institutions sponsor the DIPPR 801 Project to aid in the design and operation of their chemical processes. Sponsorship of the DIPPR 801 project ensures access to the most up-to-date version of the 801 database with the best, most accurate property values recommended. Sponsors understand that having accurate chemical data can be the difference between success and failure in chemical process design.

Sponsorships fund original research tailored to areas where the database may lack adequate values and temperature-dependent correlations. Depending on the specific need, this research may experimentally measure property data, develop and validate new or improved estimation methods, or use molecular modeling to better understand and predict property values. Generally, the results of this research are evaluated by DIPPR personnel, published in peer-reviewed literature and added to the database.

DIPPR efforts are directed by industrial needs. As sponsors submit and approve compounds to be added to the 801 database, they ensure the database contains the most industrially relevant chemicals.

Accepted Values. When adding a compound to the database, all relevant data are analyzed and evaluated by project staff, as discussed above. The evaluation process produces values and correlations considered to be the “best” for each property, meaning they meet the standards of property consistency, family trends, and other chemical information. These best values appear in the database with the “Acceptance” field marked “Accepted”. Other available data can be found in the database with different acceptance values and express the results of DIPPR’s expert review process. All Acceptance values are listed below with their attendant meanings in Table 3.

These Acceptance values are used in the database for quickly identifying which sources and values should be recommended

Table 3. Possible Values and Corresponding Meanings of Acceptance Values in the DIPPR 801 Database

acceptance value	meaning
Accepted	Indicates the value was vetted by DIPPR and found to be the most consistent and reliable value for the given property.
Rejected	The value was found to be unreliable based on DIPPR criteria and should not be recommended or used in regressing DIPPR correlations.
Not Used	This value is acceptable but is of equal or lesser accuracy than the Accepted value.
Unevaluated	This value has been entered into the database for consideration but has not yet been evaluated by DIPPR.

to users of the database. The values which do not fall under the Accepted category are kept in the database both to avoid duplicate evaluations of the same data and to allow reevaluation of data that can happen as new research or information becomes available.

An Accepted designation does not necessarily mean that the value is experimental nor that the uncertainty in the value is low. This simply means that the value reflects the most consistent and reliable information available. Accepted values can be experimental, predicted, or in the case of correlations, both. This information is clearly indicated in the database by viewing the “Data Type” field of a given property.

Uncertainty in the 801 Database. DIPPR assigns uncertainty levels to constants, temperature-dependent correlations and data sets as a percentage of the given value. These uncertainty designations are assigned by DIPPR based on data type, availability, and agreement of data sources, acquisition method, and original reported uncertainty. For predicted values, uncertainty is assigned based on general knowledge about the prediction method given the chemical family and property. The uncertainties of input properties used in prediction methods are also considered. For the sake of simplicity and to be conservative with uncertainty, DIPPR assigns nine quantized uncertainty levels to any property value. These levels are given in Table 4. Due to the quantized nature of DIPPR uncertainty levels, the reported DIPPR uncertainty will rarely be exactly the same as author estimates.

Table 4. DIPPR's Nine Quantized Uncertainty Levels

uncertainty levels (%)	
<0.2	<25
<1	<50
<3	<100
<5	>100
<10	

While DIPPR provides uncertainty levels for values and correlations, these are guidelines and still require some consideration in their use, especially if they are being used to develop new prediction methods. Uncertainty designations for temperature dependent correlations are only based on the reliability of the data that informs the correlation and not the uncertainty associated with regression. Therefore, regression statistics are also available and should be examined in addition to the quantized uncertainty. For example, it is possible that, at the edges of the given temperature range, the error of the correlation may be higher than the assigned uncertainty designation. An example of this could be vapor pressure where, at low temperatures, the true (relative) error could be orders of

magnitude larger than the assigned uncertainty. For this reason, it is recommended to examine the data sources when using a temperature-based correlation, especially near the edges of the available temperature range.

Interproperty Consistency. The analysis method DIPPR uses allows for a more holistic picture of a chemical's properties than can be found in other data sources. Many properties are dependent on other properties through thermodynamic or structural relationships. These interdependencies are illustrated in Figure 1. Analyzing these properties independently can lead to inaccuracies, so DIPPR evaluators ensure that properties are consistent with known relationships.

An example of this principle can be seen when evaluating the vapor pressure (VP), heat of vaporization (ΔH_{vap}), and liquid heat capacity (C_p^l) of a given chemical. As discussed by previous researchers,² these properties are related through the following three relationships:

$$\text{VP} = \exp\left(A + \frac{B}{T} + C\ln(T) + DT^E\right)$$

$$\Delta H_{\text{vap}} = T\Delta V \frac{d\text{VP}}{dT}$$

$$C_p^l = C_p^{\text{IG}} - T \int_0^{\text{VP}} \left(\frac{d^2V_v}{dT^2} \right) dP - \frac{d\Delta H_{\text{vap}}}{dT} + \left(\Delta V - T \left(\frac{dV_v}{dT} \right) \right) \left(\frac{d^2\text{VP}}{dT} \right)$$

Here, A , B , C , D , and E are regressed parameters, T is temperature in K, P is pressure, ΔV is the difference in volume between the vapor and liquid phases, C_p^{IG} is the ideal gas heat capacity, and V_v is the vapor volume from an equation of state.

The equations for heat of vaporization and liquid heat capacity are exact mathematical relationships and thus, the fit of the vapor pressure curve should allow prediction of the other two properties. If there are disagreements between the values, DIPPR evaluators can carefully choose the correct sources or prediction methods on which to base the DIPPR Accepted values. This also allows property information to inform other properties. Experimental data in one property can then be used to predict or verify the other two properties. These inter-relationships occur in many properties and ensuring consistency across a chemical profile improves property prediction and makes DIPPR recommendations the Gold Standard.

A useful example of using interproperty consistency to improve property prediction is illustrated by 2-decyl-1-tetradecanol, an industrially important chemical that was added to the database in 2019 (see Tables 5–8. At the time the compound was evaluated, five unique sources for vapor pressure were found, each with one data point. These values were relatively varied, had high uncertainty and were measured at low temperatures. No experimental data were available for the critical constants, heat of vaporization, or liquid heat capacity. A possible family trend was available for predicting the normal boiling point but, depending on the critical constants prediction methods, the predicted vapor pressure curve differed substantially. The spread of predictions, data, and some possible vapor pressure curves is shown in Figure 2. More information was needed.

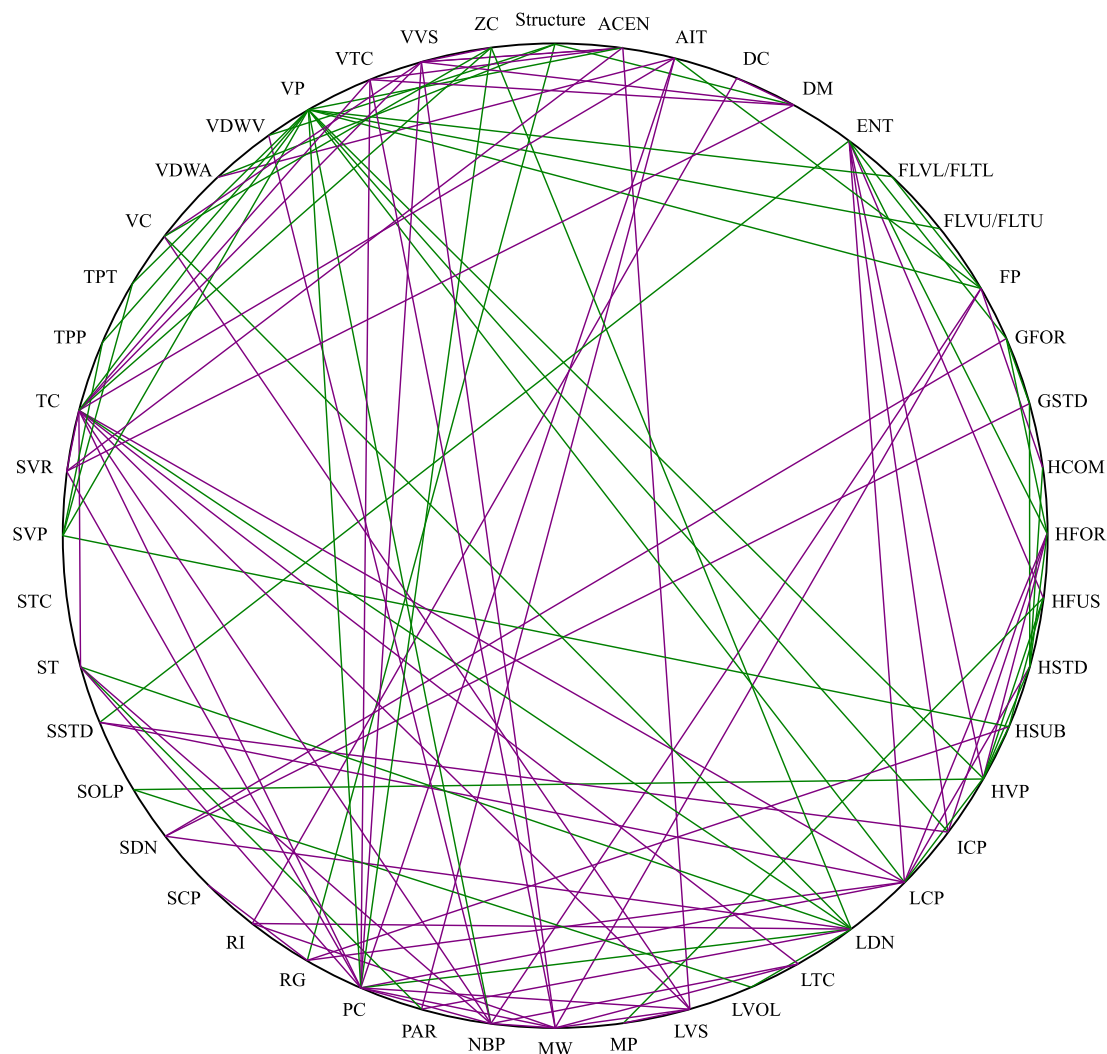


Figure 1. Interconnected properties used by the DIPPR database. Green lines show thermodynamic or rigorous relations, and purple lines show predictive equation relationships. Abbreviation meanings are shown in Tables 1 and 2. (This figure has been recreated based on Figure 1 from Rowley et al.¹)

Table 5. Experimental Vapor Pressure Data for 2-Decyl-1-tetradecanol in Figure 2

temp (K)	vapor pressure (Pa)	refs
438.15	1.33×10^{-02}	7
449.15	8.00×10^{01}	8
513.15	1.00×10^{03}	9
523.15	2.00×10^{03}	10
546.15	4.40×10^{03}	11–13

Liquid heat capacity data were measured by DIPPR personnel. By using the above thermodynamic relationships, a better correlation for the vapor pressure, heat of vaporization, and liquid heat capacity was obtained. This was done by choosing the critical constant prediction methods, normal boiling point predictions and vapor pressure data that best aligned with the measured liquid heat capacity data. By ensuring interproperty consistency, the property correlations for all three of these properties were improved. The accepted correlation can be seen in Figure 2. There are significant differences between this curve and many otherwise reasonable predictions.

Table 6. Critical Temperature Prediction Methods for 2-Decyl-1-tetradecanol in Figure 2

method	critical temperature (K)	refs
Nannoolal–TC	806.5	14
Ambrose–TC	825.8	15
Joback	825.4	16, found in 17
Lydersen	827.1	18
Wilson–Jaspersion first order	803.6	19, found in 17
Wilson–Jaspersion second order	799.7	19, found in 17
Constantinou	815.9	20
Nokay	832.7	21
Klinczewicz–Reid	795.8	22
Jalowka	749.0	23
Forman–Thodos	775.9	24

Another kind of consistency consists of comparisons to chemical family members and similar compounds. As mentioned above for 2-decyl-1-tetradecanol's boiling point, family comparisons often elucidate the best values. As many have noted, properties often follow a predictable trend in chemical families or compounds with similar structures.^{3,4}

Table 7. Critical Pressure Prediction Methods for 2-Decyl-1-tetradecanol in Figure 2

method	critical pressure (Pa)	refs
Nannoolal-PC	9.11×10^{05}	14
Ambrose-PC	1.12×10^{06}	25
Joback	8.54×10^{05}	16, found in 17
Lydersen	1.06×10^{06}	18
Wilson-Jasperson first order	8.97×10^{05}	19, found in 17
Wilson-Jasperson second order	8.97×10^{05}	19, found in 17
Constantinou	8.75×10^{05}	20
Shigaki	9.35×10^{05}	26
Klincewicz-Reid	1.19×10^{06}	22
Jalowka	1.04×10^{06}	23
Vetere	1.27×10^{06}	27, found in 28
Forman-Thodos	9.28×10^{05}	24
BYU Internal Method (VP Interpolation/Extrapolation)	9.11×10^{05}	29

Table 8. Normal Boiling Point Prediction Methods for 2-Decyl-1-tetradecanol in Figure 2

method	boiling point (K)	refs
Nannoolal	693.3	30
BYU-NBP	736.5	31
Stein	690.5	32
Constantinou	657.6	20
Joback (not shown)	840.3	16, found in 17
Meissner	695.3	33, found in ref 34
Miller	620.2	34
Pailhes	675.1	35
Modified Stein ^a	673.3	29

^aNote on the modified Stein: the Stein method predicts the normal boiling point more accurately than other methods for the 1-alcohols and other aliphatic alcohols families (1.4% average deviation and 4.2% maximum deviation). It consistently overpredicts the values for the 1-alcohols. The accepted value was obtained by subtracting 17.2 K from the value predicted with the Stein method to bring the value in line with family trends for the 1-alcohols.

With additional information about family members or similar compounds, the most correct value can be selected among several sources by comparing to data from family members and/or similar compounds. An example of this is shown in Figure 3, where vapor pressure curves of the *n*-alkanes follow a distinct pattern.

Completeness. To support sponsors' needs, DIPPR requires chemical profiles to have a complete set of values and correlations for all thermophysical properties available in the 801 Database to the maximum extent possible. DIPPR uses all the available data and existing prediction techniques to give recommendations for all the properties in the database. Specifically, DIPPR uses the most accurate estimation methods possible when reliable experimental data are unavailable. This ensures each compound has a complete set of recommendations for every constant property and temperature-dependent correlation. Thus, the 801 Database provides to users the highest likelihood of finding the value they need and avoiding frustrating blanks when looking for property values and correlations. The only exceptions are cases in which physical

properties are not applicable to a particular compound (e.g., flammability properties do not apply to water) or when no data nor reliable prediction method exists for a particular property (e.g., many compounds do not have an experimental solid thermal conductivity or available prediction method).

Dynamic Nature of the Database. Often, new data are found and entered into the database after a compound has been added and been given a complete chemical profile. When this occurs, the new data are included as Unevaluated until they can be analyzed. New data are assigned an impact factor based on the property and the time since the last review of the chemical. The impact factor also prioritizes experimental data for compounds that previously lacked such data and compounds of industrial importance. The impact factor helps DIPPR investigators know when a review of a compound is merited. This process ensures that the database stays up to date and prioritizes the most significant improvements.

Compound reviews may reassign Accepted values to reflect better information. In this way, the 801 database is a dynamic and perpetually improving database. A particular snapshot of the database will reflect the best recommendations available at that time but any property value may later be supplanted by better values as they are found and evaluated. These policies help to ensure the database remains the Gold Standard even as new data or prediction methods become available.

Common Mistakes in Publications. As the Gold Standard in chemical property data, the DIPPR 801 Database is referenced in many publications. While many researchers use the database correctly, mistakes are common in the literature. These errors often involve a fundamental misunderstanding of DIPPR's purpose and definitions. By pointing out common mistakes when using DIPPR data, we hope to avoid such problems in the future. The two most common mistakes include interpreting DIPPR Accepted constant values and temperature-dependent correlations as experimental data and neglecting to properly credit original data sources. Specific examples from the literature appear below.

Insufficient Citations. In a recent article, a neural network model for surface tension collected data from DIPPR, DETHERM, and additional works.⁵ The method reported an excellent fit to 3063 data points on 149 alcohols. While the authors have carefully noted the number of data points collected for each compound in an appendix along with the used physical properties, they neglected to cite the experimental data and physical property data sources. While they do cite the edition of the databases they use, referencing the original data sources would allow researchers to better analyze and review their work by allowing scrutiny of the primary data.

Treating DIPPR values as a primary source is a frequent mistake in the literature. Many values in the database are predicted, smoothed, or may be cited from another source in the literature. By neglecting to reference the original data in this case, it is unclear whether the values used in fitting are from a primary source or some other source that is either predicted, smoothed, or repeats some value from a primary source. This can invalidate claims made by the author about how well the method fits to experimental data. These problems can be avoided by referencing the original sources where possible.

Using Correlation Values as Experimental. Temperature-dependent properties are presented as correlations in the database to make simulation and process design easier.

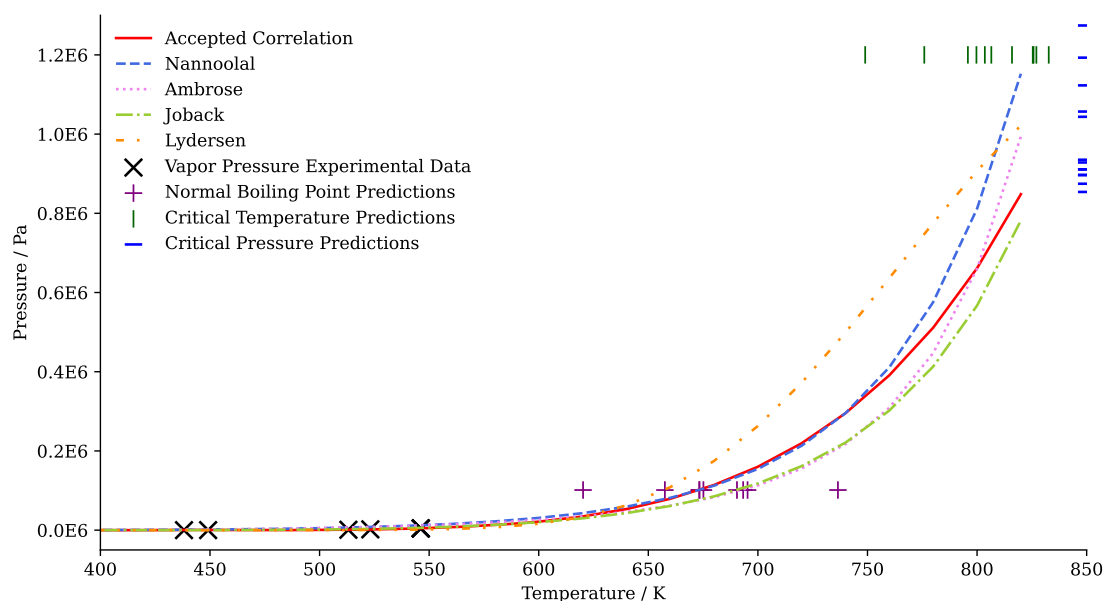


Figure 2. Some potential vapor pressure curve predictions for 2-decyl-1-tetradecanol before liquid heat capacity data were available for consistency checks. Critical temperature predictions from 11 methods are plotted at an arbitrary pressure of 1 200 000 Pa for comparison and 13 critical pressure predictions plotted at arbitrary temperature of 850 K for comparison. Normal boiling point predictions from nine methods are shown and experimental VP data from five sources are plotted as well. Nannoolal line uses Nannoolal predictions for TC and PC and primary NBP prediction method to fit Riedel VP curve, Ambrose line uses Ambrose predictions for TC and PC and secondary NBP prediction method to fit Riedel, and so on with Joback and Lydersen curves. Many more lines are possible as the TC, PC, and NBP used for regression are changed. Data, values, and sources can be found in the appendix.

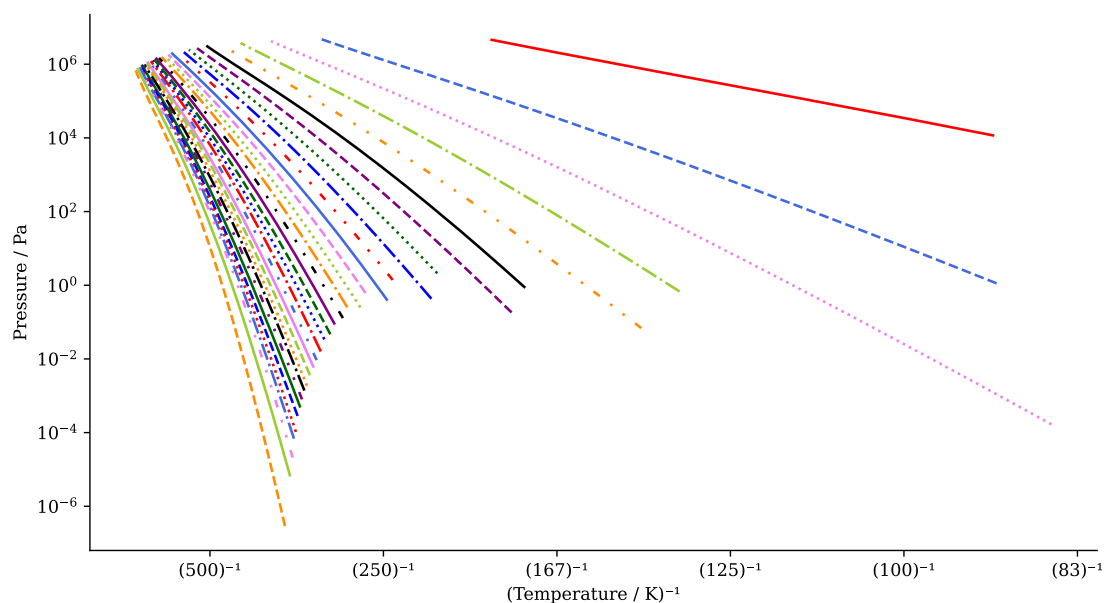


Figure 3. DIPPR-accepted vapor pressure correlations for the *n*-alkane family. Species proceed with decreasing carbon number from *n*-hexatriacontane (orange and dashed, far left) to methane (red and solid, far right). Not all possible species are present.

However, researchers have often treated values from correlations as experimental data points. DIPPR recommended correlations can be regressed from multiple data experimental sources and/or prediction methods. The type of data used in the regression is fully noted in the database, but researchers often neglect to consider this. When used for comparisons, data sources and regression information should be shared as well. For compounds with sufficient experimental data, the DIPPR correlations are highly accurate. Where fewer experimental data are available, correlations are regressed based on the best prediction methods available. However,

these correlations tend to have greater uncertainty. Therefore, treating correlation results as experimental data may be inaccurate depending on the data that informed the correlation fit. This problem may be avoided by checking and referencing the sources that informed the correlation.

Interpreting Recommended Values as Experimental.

In a 2018 article, Keshavarz et al. published a quantitative structure–property relationship (QSPR) for the prediction of autoignition temperatures (AIT).⁶ In it, they claim to use experimental data for 54 compounds to relate molecular descriptors to AIT. However, upon closer inspection, 19 AIT

values they attribute to the DIPPR database are predicted rather than experimental values. The authors incorrectly included Accepted values without examining whether the values were experimental. This neglect calls into question the entire prediction method because the regression is based on predicted values.

Researchers can easily avoid this situation. DIPPR includes information for every recommended value to identify its origin and whether it is an experimental or predicted value. Researchers should screen the data they use for new prediction methods to avoid using nonexperimental values.

How to Correctly Report DIPPR Values. Correctly using and citing DIPPR values can make data collection and processing easier as well as increase the legitimacy of published findings. So far, common mistakes in the literature have been discussed and DIPPR processes have been explained. With this information, a discussion of best practices for authors and reviewers is appropriate. Following these suggested best practices will ensure the database is interpreted correctly and is most useful to any who access it.

Understand Data Type. Before using values collected from DIPPR, make sure the Data Type selected is appropriate for your application. All of DIPPR's available data types and a brief description are shown in Table 9. For process design, the

Table 9. Data Type Designations and Their Corresponding Meanings in the DIPPR 801 Database

data type	meaning
Experimental	Data corresponding to experimental results
Predicted	Data points using prediction methods
Exp&Pred	Experimental and predicted data
Defined	A constant value defined by an equation
Derived	Value calculated from well-established thermodynamic relationships using other properties
Smoothed	Interpolated or smoothed data
Not Specified	Values reported with no indication of how they were obtained

Accepted DIPPR value is the best choice and is the central use case for the database. For creating prediction methods, parametrizing group contribution methods, or other scientific work, use only values that are based on experimental data. DIPPR software and tools make this easy by allowing database searches based on Data Type. If Accepted values are used for creating new estimation methods without reference to Data Type, there is a risk of only replicating the effectiveness of past methods rather than building new ones. This sort of error can introduce unforeseen uncertainty or even invalidate an estimation method.

Reference Original Source. When using values or correlations from the DIPPR 801 database, cite DIPPR appropriately. Additionally, reference the primary source including the original author or method used. The 801 database includes the source of each value or correlation where possible. Using the primary source will ensure the property values are understood and reviewed in their original context. This often allows a lower uncertainty to be assigned to property values. Primary source use will also improve transparency in published papers and allow for proper credit to be given to original researchers. Finally, this will also allow more meaningful comparisons between researchers and measurement methods.

In some cases, DIPPR uses internal methods to produce Predicted, Defined, or Derived values in the database. Where DIPPR has produced values using internal methods, DIPPR should be directly referenced. The database will clearly indicate these values as having been produced via an internal method. While these values are not experimental data, they represent the best property estimates available. Cite these values as a DIPPR recommended value based on internal methods.

The appropriate citation is listed as the following. As principal investigators change and years progress, update this reference accordingly: Wilding, W. V.; Knotts, T. A.; Giles, N. F.; Rowley, R. L. *DIPPR Data Compilation of Pure Chemical Properties*; Design Institute for Physical Properties, AIChE: New York, NY, 2020.

Check Uncertainty. As discussed previously, to simplify the database and allow for staff insight into data reliability, DIPPR uncertainty designations are quantized. This is often not representative of the exact uncertainty that may be obtained from the original source of the value or correlation. Often for correlations, the uncertainty may be much lower than the DIPPR-assigned uncertainty in temperature regions that include experimental data.

Additionally, Accepted values and correlations do not imply low uncertainty. Although a data point or a correlation may be Accepted, the data point or correlation for a given property could have a large uncertainty. When using values, consider the uncertainty and the needs of the application. This practice can inform whether more exact predictions or data should be obtained, such as before a large capital investment.

Examine Correlation Limitations. When using DIPPR recommended correlations, ensure the temperature range of the correlation is representative of the application and avoid using any correlation outside of its stated temperature range. As discussed previously, the uncertainty assigned to a correlation is based on the data informing the correlation and regression uncertainty is still possible. Therefore, correlation values far from experimental data can have a much higher error than the assigned uncertainty level. For these reasons, checking the value sources and regression statistics is important. Finally, use caution when using a correlation near the edges of its temperature range.

CONCLUSION

We have discussed DIPPR terminology, DIPPR evaluations and processes, common mistakes in using DIPPR resources, and best practices in using DIPPR in scientific work. DIPPR is committed to maintaining the 801 database as the Gold Standard for pure-component physical property data. Using DIPPR's proprietary methodology ensures the best results to be recommended to professionals. The usage recommendations herein will (if followed) ensure the correct use of DIPPR values, leading to more meaningful and transparent publications for engineers and scientists everywhere.

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<https://pubs.acs.org/10.1021/acs.jced.0c00641>

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Notes

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