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Beom Chan Ryu

Korea University

Sun Yoo Hwang

Korea University

Chang Geun Kim

National Center for Standard Reference Data (NCSRD)

Jeong Won Kang

`jwkang@korea.ac.kr`

Korea University

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Title page

Title

Integrated Evaluation Framework for Standard Reference Thermophysical Property Data in the Korean Thermophysical Properties Databank (KDB)

Author information

Beom Chan Ryu¹, Sun Yoo Hwang¹, Chang Geun Kim², Jeong Won Kang^{1*}

¹ Department of Chemical and Biological Engineering, Korea University, Seoul 02841, Republic of Korea

² National Center for Standard Reference Data (NCSRD), Daejeon 34113, Republic of Korea

* *Corresponding author.* (jwkang@korea.ac.kr)

Abstract

Reliable thermophysical property data requires both accurate measurement and transparent evaluation of uncertainty and source traceability. Although the Korean Thermophysical Properties Databank (KDB) has previously provided critically evaluated data, the evaluation workflow for standard reference data has not been described as a coherent and reproducible procedure. In this study, a structured framework for constructing standard reference data within the KDB is formalized and validated. The procedure integrates traceable data collection, iterative outlier rejection, uncertainty evaluation and propagation, independent cross-checking, and expert committee review into a unified evaluation process. This methodology was applied to six thermophysical properties relevant to process design, safety, and environmental assessment: flash point, octanol–water partition coefficient, autoignition temperature, surface tension, acentric factor, and Hildebrand solubility parameter. Applying the evaluation to 82,488 raw literature data points resulted in 2,363 registered standard reference data entries. Cross-checking against independent comparison values provided the evidentiary basis for the registration decisions and revealed errors in supporting database entries. The evaluated data have been incorporated into the publicly accessible KDB platform, together with metadata including uncertainty estimates and quality classifications. This framework establishes a systematic methodology for consolidating heterogeneous literature data into uncertainty-aware standard reference data.

Keywords

Thermophysical property, Standard reference data, Data evaluation, Uncertainty, Cross-checking, Traceability

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Competing interests

The authors have no financial or competing interests to declare that are relevant to the content of this article.

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Data availability statements

All evaluated property values, together with their uncertainties and quality classifications, are available in the KDB platform (<https://www.mdlkdb.com>).

CRedit authorship contribution statement

Beom Chan Ryu: Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft. **Sun Yoo Hwang:** Data curation, Formal analysis, Software. **Chang Geun Kim:** Conceptualization, Validation. **Jeong Won Kang:** Methodology, Supervision, Writing – review & editing.

1. Introduction

High-quality thermophysical data are essential for engineering and scientific applications. Reliable property data are required to validate theoretical models, identify physical trends, and improve the performance of property prediction methods [1, 2]. The reliability depends not only on the reported property values but also on the associated measurement uncertainty, which quantifies confidence in the measurements. In process design, uncertainty influences equipment sizing, operating margins, and mass and energy balance calculations [3, 4]. In process safety, reliable kinetic and thermodynamic properties are necessary for safety-valve design and fire hazard assessment [5, 6]. In environmental risk assessment, uncertainty in fundamental thermodynamic quantities propagates directly into calculated environmental indicators, making traceable uncertainty estimates essential for defensible risk assessment [7]. Therefore, uncertainty information is indispensable for assessing data quality and establishing trustworthy process design.

Most existing thermophysical databases prioritize either broad accessibility or rigorous uncertainty evaluation. Open databases and software packages, such as CoolProp [8] and OpenCalphad [9], provide extensive public access to thermophysical property information, but do not yet include systematic uncertainty quantification as a standard feature. In contrast, critically evaluated resources such as DIPPR [10, 11], NIST ThermoData Engine (NIST-TDE) [12, 13], and REFPROP [14] incorporate uncertainty information directly into their data evaluation frameworks, but are mainly available through subscription or licensing models. Some freely accessible databases, including ILThermo [15] and the nanofluid database [16], show that open access and uncertainty reporting can coexist. However, these initiatives are limited to specific compound classes or applications. As a result, there remains a need for an openly accessible thermophysical database that combines broad property coverage with

systematic, uncertainty-based data evaluation.

Previous work relaunched the Korean Thermophysical Properties Databank (KDB) web platform, making critically evaluated data available for approximately 1,970 compounds and 5,567 binary vapor–liquid equilibrium data sets [17]. This release implemented a general-purpose evaluation framework that grades property values on a five-level scale based on accuracy, reproducibility, and consistency. The framework uses statistical outlier rejection and cross-validation with a group-contribution-based graph convolutional network (GC-GCN) [18, 19]. However, the platform-level description did not document the individual components underlying each entry, including source traceability, outlier rejection, uncertainty estimation, model-based cross-checking, and expert committee registration decisions, as a coherent and reproducible evaluation procedure.

This study formalizes and validates the construction of standard reference data using an evaluation framework that is both uncertainty-aware and traceability-preserving. The framework integrates traceable data collection, iterative $\pm 2\sigma$ outlier rejection, uncertainty evaluation, uncertainty propagation, independent cross-checking, and expert-committee review into a single systematic workflow. Its applicability is demonstrated for six thermophysical properties relevant to safety, environmental assessment, and process design: flash point (FP), octanol–water partition coefficient ($\log K_{ow}$), autoignition temperature (AIT), surface tension (γ), acentric factor (ω), and Hildebrand solubility parameter (δ). Together, these components provide a practical methodology for generating high-quality standard reference data and ensuring broad public accessibility through the KDB platform.

2. Methodology

Fig. 1 provides an overview of the workflow used to construct standard reference data. The framework consists of three phases: traceable data collection and refinement (Section 2.1); data evaluation, including outlier screening, uncertainty evaluation, and cross-checking with independent comparison values (Sections 2.2 to 2.4); and expert committee review followed by registration in the KDB platform (Section 2.4). Each phase is described in detail in the following subsections.

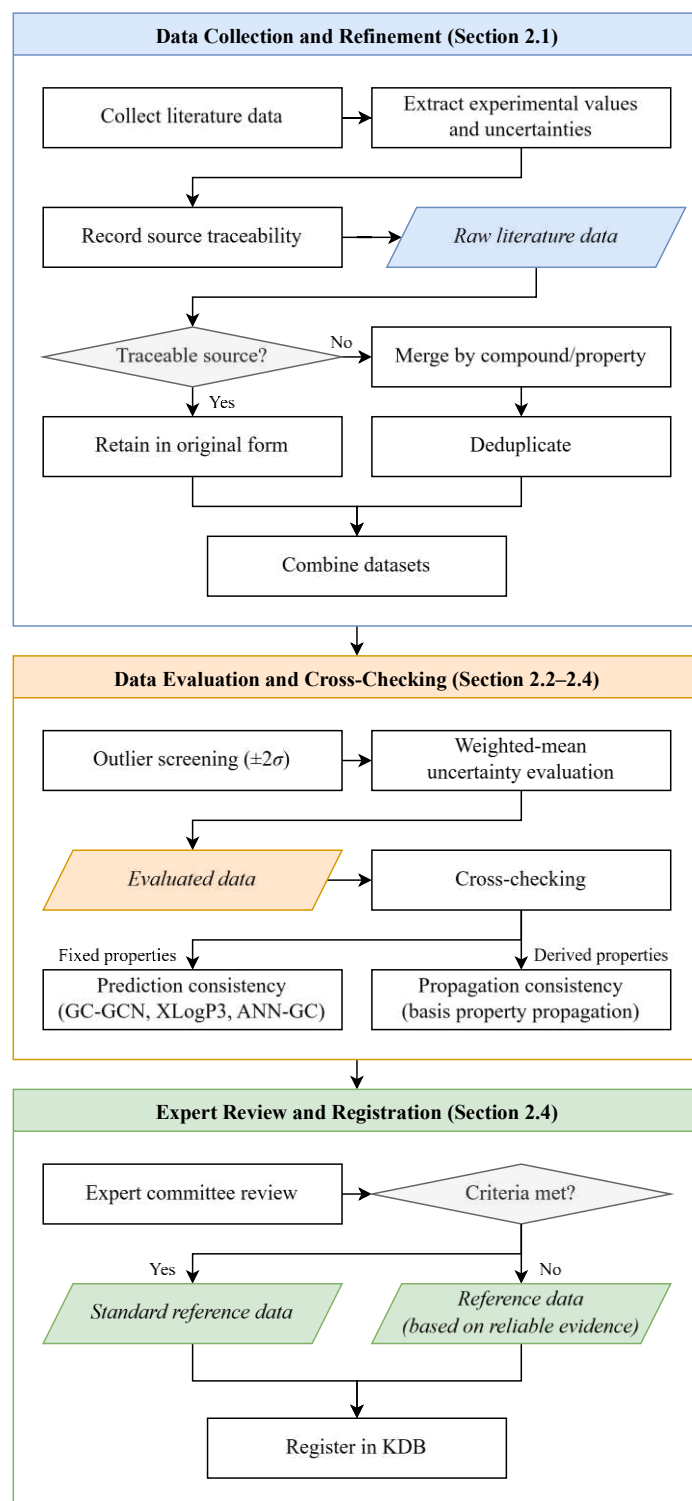


Fig. 1 Overall workflow of the proposed framework, consisting of data collection and refinement, data evaluation and cross-checking, and expert review and registration.

2.1. Data Collection and Refinement

Data for six thermophysical properties were collected: flash point (FP), octanol–water partition coefficient ($\log K_{ow}$), autoignition temperature (AIT), surface tension (γ), acentric factor (ω), and Hildebrand solubility parameter (δ). For surface tension and Hildebrand solubility parameter, literature data reported at 298.15 K were used. Sources included peer-reviewed literature, standard reference compilations, and the original KDB dataset [10, 13, 20–60]. For Hansen parameter data, the total solubility parameter was calculated as $\delta = \sqrt{\delta_D^2 + \delta_P^2 + \delta_H^2}$ and used as the Hildebrand solubility parameter. A total of 82,488 raw data points were compiled, with up to 15 sources contributing to each property (Table 1). The original reference for each data point was identified and recorded to maintain traceability to the source publication.

Before uncertainty evaluation, the raw literature data were deduplicated based on the traceability of their sources. Sources were classified as traceable if each reported value could be linked to a specific experiment or publication. Traceable sources were retained in their original form to preserve the complete set of reported measurements for subsequent uncertainty evaluation. Sources were classified as non-traceable if they provided values that had already been statistically aggregated across multiple studies, such as a single averaged value per compound without individual source attribution. Non-traceable sources were merged by compound and property, then deduplicated, assuming these values might already reflect prior aggregation. The refined non-traceable dataset was then combined with the traceable dataset to form the dataset used for outlier detection and uncertainty evaluation.

Table 1 Sources of raw literature data collected for six thermophysical properties

Property	Number of sources	Sources
Flash point (FP)	12	[10, 20-30]
Octanol–water partition coefficient ($\log K_{ow}$)	14	[23, 31-43]
Autoignition temperature (AIT)	15	[10, 20, 23, 44-55]
Surface tension (γ)	3	[10, 13, 23]
Acentric factor (ω)	3	[10, 56, 57]
Hildebrand solubility parameter (δ)	3	[58-60]

2.2. Uncertainty Evaluation of Properties

The deduplicated data points for each compound across the six properties were evaluated in two stages: outlier detection and weighted-mean uncertainty estimation.

Outlier detection was performed for compounds with at least six data points using an iterative z-score criterion. At each step, the arithmetic mean and standard deviation were recalculated for the remaining data. Data points with $|z| > 2$ were removed, and this process continued until all remaining points satisfied the criterion. This procedure defines a $\pm 2\sigma$ (four-sigma-wide) acceptance range, which is more restrictive than the $\pm 3\sigma$ (six-sigma-wide) range used in previous studies [17]. The $\pm 2\sigma$ range was chosen because thermophysical property databases typically contain few data points per compound. For a sample of size N , the maximum possible z-score limits the effectiveness of the criterion; a $\pm 3\sigma$ threshold can only identify outliers when $N \geq 11$, whereas the $\pm 2\sigma$ threshold becomes effective at $N \geq 6$. Compounds with fewer than three data points were not evaluated further, as reliable consensus could not be established with so few measurements. Compounds with three to five data points were carried forward to weighted averaging without outlier screening.

Each retained data point x_i was assigned to an inverse-variance weight according to its reported standard uncertainty, u_i .

$$w_i = \frac{1}{u_i^2} \quad (1)$$

When reported uncertainties were unavailable, estimated uncertainties were assigned based on the average reported experimental uncertainty. To address variations in source reliability, the average value was applied to measurements from traceable literature sources, while twice the average value was assigned to data from sources with limited traceability as a penalty. For fixed properties, the assigned standard deviations were 1.7 K for FP, 0.050 for $\log K_{ow}$, and 1.2 of the

reported AIT. For data from sources with limited traceability, these values were doubled. For derived properties, uncertainties were taken directly from the KDB, DIPPR, and NIST sources when available, and no additional uncertainty was estimated; data points for which no uncertainty was available were excluded from the weighted mean.

All weights were normalized so that their sum was equal to one. To limit the influence of any single data point with a very small, reported uncertainty, the maximum relative weight was set to 0.5. Where this cap was active, the affected weight was fixed at 0.5 and the weights of the remaining points were rescaled so that they summed to 0.5; the step was repeated until no weight exceeded the cap. The adjusted weights therefore sum to unity and no single measurement contributes more than half of the weighted mean.

$$\hat{w}_i = \min\left(0.5, \frac{w_i}{\sum_i w_i}\right) \quad (2)$$

The weighted mean (x_w) and its standard uncertainty (u_w) were then calculated using these adjusted weights.

$$x_w = \sum_i^N \hat{w}_i x_i \quad (3)$$

$$u_w = \sqrt{\sum_i^N \hat{w}_i^2 u_i^2} \quad (4)$$

The chi-squared statistic was calculated using the reported or assigned standard uncertainty.

$$\chi^2 = \sum_i^N \frac{(x_i - x_w)^2}{u_i^2} \quad (5)$$

From this statistic, the Birge ratio was obtained as follows:

$$R_B = \sqrt{\frac{\chi^2}{N-1}} \quad (6)$$

The combined standard uncertainty was scaled using the Birge ratio only if $R_B > 1$.

$$u = u_w \times \max(1, R_B) \quad (7)$$

Each evaluated data entry was reported with its expanded uncertainty, using a coverage factor of $k = 2$. The number of significant digits for each value was determined by the leading significant digit of the uncertainty, unless this exceeded the precision of the original data.

2.3. Uncertainty Propagation for Derived Properties

Data for the three derived properties considered in this study—surface tension (γ), the acentric factor (ω), and Hildebrand solubility parameter (δ)—were compiled from the literature according to the procedure described in Section 2.1. To provide independent validation of these aggregated values, each derived property was also estimated by propagating the uncertainties of its fundamental basis properties through the relevant defining or correlating equation.

The basis properties and their associated uncertainties used for uncertainty propagation were obtained from several sources, as summarized in Table 2. The critical temperature and critical pressure, which are required for both γ and ω , were obtained from the original KDB dataset [58]. The enthalpy of vaporization and liquid density, required for δ , were obtained from DIPPR [10] and NIST-TDE [13], with supplementary data from Acree’s publications [61, 62]. Liquid densities were converted to molar volumes using the molecular weight of each compound. Both γ and δ are temperature-dependent, and all evaluated values, propagated estimates, and basis properties reported in this work refer to a common reference temperature of 298.15 K. Literature values reported at other temperatures were excluded.

Correlation coefficients for vapor pressure, used in the calculation of ω , and for the surface tension were obtained from DIPPR [10] and Yaws [57].

Surface tension was calculated using the correlation equation provided by DIPPR [10].

$$\gamma = A(1 - T_r)^{(B+CT_r+DT_r^2+ET_r^3)} \quad (8)$$

In this equation, $T_r = T/T_c$ is the reduced temperature, and A – E are compound-specific coefficients. Of the variables in Eq. (8), only the critical temperature T_c was treated as an uncertain basis property. The coefficients A – E were treated as fixed constants because their uncertainties were not reported in the source. Therefore, uncertainty propagation was

performed only with respect to T_c .

$$u_\gamma = \left| \frac{\partial \gamma}{\partial T_c} \right| u_{T_c} \quad (9)$$

The acentric factor was defined according to Pitzer [63].

$$\omega = -\log_{10}(p_r^{vap}|_{T_r=0.7}) - 1 \quad (10)$$

The reduced saturation vapor pressure (p_r^{vap}) at $T_r = 0.7$ was determined using a vapor pressure correlation [64].

$$\ln p^{vap} = A + \frac{B}{T} + C \ln T + DT^E \quad (11)$$

The coefficients A – E were also treated as fixed constants, consistent with the approach used for γ , because their uncertainties were not reported. Critical temperature and critical pressure were considered the basis properties with associated uncertainty. Partial derivatives of ω with respect to T_c and p_c were calculated by differentiating Eqs. (9) and (10) with respect to each basis property. The propagated uncertainty was then determined as described below.

$$u_\omega = \sqrt{\left(\frac{\partial \omega}{\partial p_c} \right)^2 u_{p_c}^2 + \left(\frac{\partial \omega}{\partial T_c} \right)^2 u_{T_c}^2} \quad (12)$$

The Hildebrand solubility parameter was defined as follows [65].

$$\delta = \sqrt{\frac{\Delta_{vap}H - RT}{V_m}} \quad (13)$$

In Eq. (13), R is the gas constant, and the basis properties are the enthalpy of vaporization ($\Delta_{vap}H$) and the molar volume (V_m). The propagated uncertainty was calculated as follows.

$$u_\delta = \sqrt{\left(\frac{\partial \delta}{\partial \Delta_{vap}H} \right)^2 u_{\Delta_{vap}H}^2 + \left(\frac{\partial \delta}{\partial V_m} \right)^2 u_{V_m}^2} \quad (14)$$

Table 2 Sources of basis properties and correlation coefficients used for uncertainty propagation

Basis property	Used in	Source(s)
Critical temperature (T_c)	γ, ω	[58]
Critical pressure (p_c)	ω	[58]
Enthalpy of vaporization ($\Delta_{\text{vap}}H$)	δ	[10, 13, 61, 62]
Liquid density (for molar volume)	δ	[10, 13, 61, 62]
Vapor pressure correlation coefficients	ω	[10, 57]
Surface tension correlation coefficients	γ	[10, 57]

2.4. Cross-checking and Registration Procedure

Prior to expert evaluation, each value was independently cross-checked against a comparison value derived from an external predictive model or an independent propagation calculation, depending on the property type. This comparison supplies the evidence for one criterion in Table 3 (Criterion 8 for fixed properties, Criterion 6 for derived properties) so that seven of the eight criteria apply to any given value, regardless of property type. A value was registered as standard reference data only when all seven applicable criteria were satisfied, meaning a failed cross-check alone was sufficient to prevent registration. This study used a single cross-checking method for each property type (predictive model comparison for fixed properties and propagation-based comparison for derived properties).

For the three fixed properties, the weighted-mean values from Section 2.2 were compared with predictions from established group-contribution or machine-learning models: the GC-GCN model for FP [18], the XLogP3 model for $\log K_{ow}$ [66], and the ANN-GC model for AIT [67]. These comparisons provide the evidentiary basis for Criterion 8 in Table 3, which requires that the evaluated data follow a reasonable trend relative to a well-established predictive model rather than match the model prediction exactly.

For the three derived properties, the evaluated data from Sections 2.1 and 2.2 were compared with propagated estimates calculated from the corresponding basis properties using the equations in Section 2.3. These comparisons provide the evidentiary basis for Criterion 6, which requires that the evaluated data agree, within their uncertainty, with a value independently obtained from an established theoretical relationship.

After cross-checking, the expert committee assessed each candidate value against the eight criteria in Table 3. These criteria address the definition and purpose of the measurand; the adequacy of the measurement method and procedure; traceability; the appropriateness of the

uncertainty evaluation; consistency with theoretical values (Criterion 6, for derived properties); consistency with literature values; and correlation with related characteristics (Criterion 8, for fixed properties).

Because exactly seven of the eight criteria apply to any given value in this work, a value was registered as standard reference data only when all seven applicable criteria were satisfied. Data that did not meet this threshold were generally retained as reference data if the underlying experimental evidence was considered reliable. While the KDB platform continues to use the previously established five-level grading system (grade 1 being the lowest and grade 5 the highest) [17], this study adopts a two-level classification to more directly represent the outcome of the evaluation procedure. Registered standard reference data correspond to grades 2–5 of that five-level system and reference data to grade 1, so that values retrieved from the KDB platform can be mapped onto the classification used here. The expert committee comprised six members with expertise in thermodynamics. Each procedure and candidate value was assessed by the committee members, and disagreements were resolved by consensus discussion.

Table 3 Expert committee evaluation criteria for the registration of standard reference data

No.	Criterion	Fixed properties	Derived properties
1	Measurand and purpose clearly defined	✓	✓
2	Measurement method adequately described	✓	✓
3	Measurement procedure adequately described	✓	✓
4	Traceability established	✓	✓
5	Uncertainty evaluation appropriate	✓	✓
6	Consistency with theoretical values	—	✓
7	Consistency with literature values	✓	✓
8	Correlation with related characteristics	✓	—

3. Results and Discussion

3.1. Dataset Statistics

Table 4 provides a stepwise summary of the data-processing pipeline for each property. The process begins with the raw literature data points collected in Section 2.1. It proceeds by removing duplicates, excluding compounds with fewer than three data points, rejecting outliers, and consolidating into compound-specific values. The final stage is the classification of these values into standard reference data and reference data.

After uncertainty evaluation and expert committee review, 2,363 compound-specific standard reference data were established and registered in KDB. The remaining 1,198 evaluated values were retained as reference data. Each registered value, whether standard reference data or reference data, represents a single compound-specific estimate. This estimate was obtained by merging the literature-reported measurements that passed all screening stages using weighted-mean estimation. As a result, these entries do not correspond to individual experimental measurements in isolation.

The relative impact of each data removal stage varied by property. For $\log K_{ow}$, excluding compounds with fewer than three data points accounted for most of the reduction, with 26,584 of the 40,258 points removed during deduplication and $N < 3$ rejection. This shows the large number of compounds represented by only one or two sources after removing duplicate entries from overlapping QSAR- and QSPR-based compilations. Outlier rejection removed a small fraction of the remaining points at each property, ranging from 0.21% for $\log K_{ow}$ to 5.36% for γ . This is consistent with the intended use of the $\pm 2\sigma$ criterion to identify a small number of clearly discordant values rather than substantially reduce the dataset.

The consolidation rate, defined as 100 times the number of standard reference data divided by the number of raw literature data points, ranged from 0.80% for $\log K_{ow}$ to 8.89% for

acentric factor. This variation mainly reflects differences in the composition and redundancy of the underlying literature, rather than differences in the evaluation procedure. The low consolidation rate for $\log K_{ow}$ was due to the inclusion of several large QSAR- and QSPR-based compilations that covered many of the same compounds. This led to extensive duplicate removal and, after consolidation, to a large number of compounds falling below the $N < 3$ threshold.

These results show that a heterogeneous collection of literature data can be systematically integrated into a set of standard reference data using the proposed evaluation procedure, with Table 4 making explicit at which stage of the pipeline each property's data were reduced.

Table 4 Data-processing pipeline from raw literature data points to standard reference data and reference data, by property

Data processing	Flash point (FP)	Octanol-water partition coefficient (log K_{ow})	Autoignition temperature (AIT)	Surface tension (γ)	Acentric factor (ω)	Solubility parameter (δ)	Total
Raw data points (data points)	20,155	44,961	8,669	3,656	4,286	761	82,488
Deduplication (data points)	16,491 (-3,664)	31,287 (-13,674)	6,916 (-1,753)	2,791 (-865)	3,715 (-571)	716 (-45)	61,916
$N < 3$ rejection (data points)	9,475 (-7,016)	4,703 (-26,584)	5,748 (-1,168)	1,231 (-1,560)	1,398 (-2,317)	458 (-258)	23,013
Outlier rejection (data points)	9,380 (-95)	4,693 (-10)	5,690 (-58)	1,165 (-66)	1,370 (-28)	443 (-15)	22,741
Evaluated data ^a (compounds)	1134	622	649	421	397	338	3,561
Standard reference data (compounds)	854	361	413	294	381	60	2,363
Reference data (compounds)	280	261	236	127	16	278	1,198
Consolidation rate (%) ^b	4.24	0.80	4.76	8.04	8.89	7.88	2.86

^a Evaluated data = Standard reference data + Reference data.

^b Consolidation rate (%) = $100 \times \text{Standard reference data} / \text{Raw data points}$.

3.2. Cross-checking Results

The thermophysical property values summarized in Section 3.1 were established using the evaluation framework described in Section 2. This framework includes uncertainty evaluation, cross-checking, and expert committee review. Cross-checking serves two main functions. First, it supports registration decisions by evaluating consistency with independent comparison methods. Second, it acts as a diagnostic tool to detect potential inconsistencies within the database. The following section presents the cross-checking results in detail.

The cross-checking procedure distinguishes between fixed and derived properties, reflecting their specific roles in the KDB framework. For the three fixed properties (FP, $\log K_{ow}$, and AIT), evaluated data were compared with established predictive models that represent general structure–property relationships, as described in Criterion 8 of Section 2.4. For the three derived properties (γ , ω , and δ), evaluated data were compared with values independently calculated by propagating the uncertainties of their basis properties through the defining equations, as specified in Criterion 6. Although the comparison methods differ, both approaches provide an independent assessment of the consistency of the evaluated data.

In both cases, a data point satisfied the cross-checking criterion if the expanded uncertainty interval ($k = 2$) of the evaluated data overlapped with that of the comparison value. For fixed properties, the comparison value was a model prediction. For derived properties, it was a propagated estimate. Data points that met this overlap criterion also met the corresponding expert evaluation criterion. Data points that did not meet the overlap criterion were retained as reference data because they had already passed statistical evaluation and originated from reliable experimental sources. Therefore, disagreement in cross-checking indicates inconsistency with an independent reference, not unreliability of the measurement.

Fig. 2 shows the cross-checking results for FP, $\log K_{ow}$, and AIT, using the GC-GCN [18],

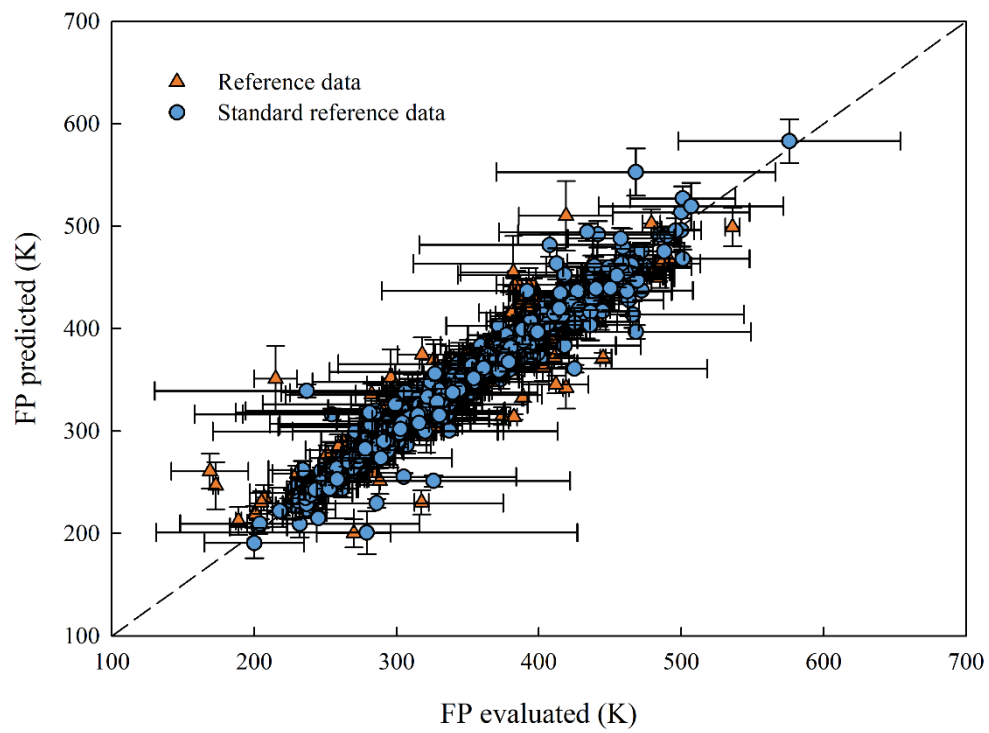
XLogP3 [66], and ANN-GC models [67], respectively. For all three properties, the standard reference data are closely clustered around the parity line, while the reference data display greater scatter. This separation requires careful interpretation, because agreement with the predictive model is one of the registration criteria (Criterion 8). Values that deviate from the model prediction are less likely to be registered as standard reference data. As a result, Fig. 2 demonstrates the internal consistency of the registration procedure rather than providing an independent validation of the retained dataset. For example, the GC-GCN model was developed using data that overlap with those in the present compilation [18], so the observed agreement for FP does not represent a fully independent test.

Fig. 3 presents the comparisons of γ , ω , and δ with the propagation estimates. In addition to supporting registration decisions, cross-checking serves as a diagnostic tool to identify inconsistencies in the original KDB dataset. For the acentric factor, ethylcyclohexane showed an unusually wide propagated uncertainty (-0.320 to 1.891), which allowed the overlap criterion to be satisfied despite a clear difference between the two central estimates. Further analysis showed that the propagation calculation used a critical temperature of 546 ± 120 K from the original KDB dataset [58], whereas the NIST Chemistry WebBook reports 609 K [68]. The uncertainty in the propagated acentric factor depends strongly on the uncertainty in the critical temperature. As a result, this basis property significantly increased the propagated uncertainty and masked the discrepancy between the two central estimates. Another inconsistency was found in the Hildebrand solubility parameter. The propagated estimates for water ($47.92 \pm 0.01 \text{ MPa}^{0.5}$) and ethyl iodide ($19.05 \pm 0.01 \text{ MPa}^{0.5}$) closely matched literature values (47.9 and $19.2 \text{ MPa}^{0.5}$, respectively) [69]. In contrast, the original KDB entries were 12.44 and $38.33 \text{ MPa}^{0.5}$ [58], indicating errors in the stored database values rather than disagreement between experiment and theory. These examples show that cross-checking can identify both inconsistent evaluated data and errors in supporting database entries, providing

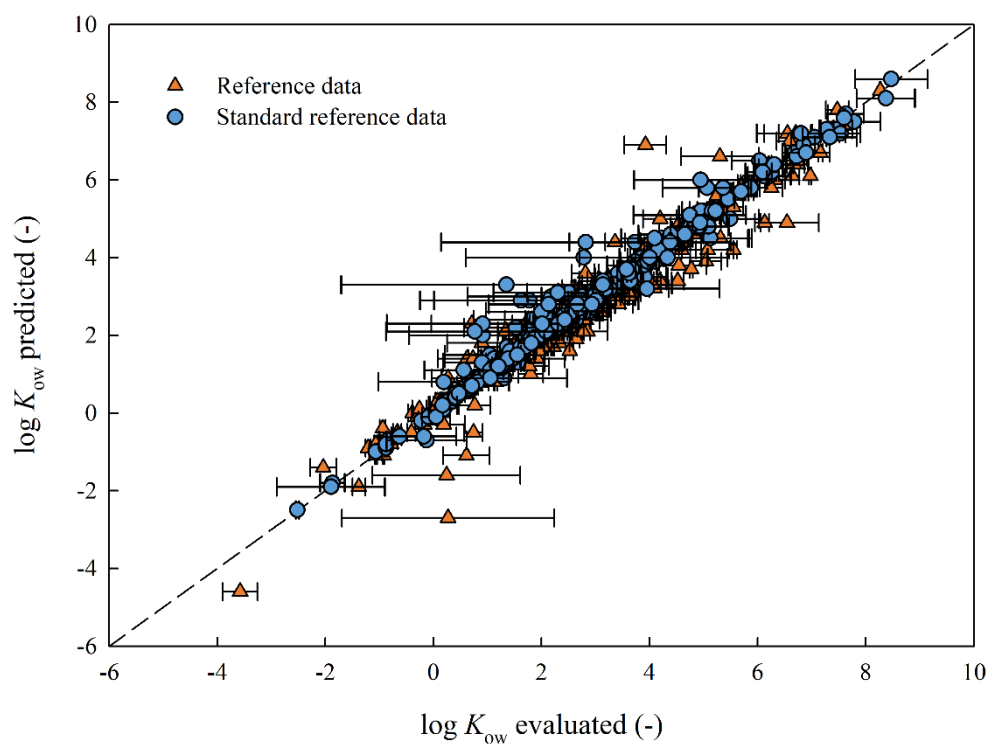
an additional layer of quality assurance beyond the formal registration criteria. The identified discrepancies in the KDB entries will be reviewed and corrected in a future KDB update.

Table 5 presents the quantitative agreement between the evaluated data and their corresponding comparison values. The metrics used are mean absolute error (MAE) and coefficient of determination (R^2), reported separately for the total evaluated data, the standard reference data, and the reference data. For five of the six properties, the standard reference data exhibit both lower MAE and higher R^2 than the reference data. This outcome is consistent with the prioritization of standard reference data during registration. The acentric factor (ω) is the exception. Its standard reference data yield a lower R^2 (0.9232) than both the reference data (0.9747) and the overall evaluated data (0.9261), though the reference data R^2 is based on only 16 compounds and is therefore statistically unstable. This difference is primarily attributable to the ethylcyclohexane data point discussed above. Excluding this single compound increases the R^2 from 0.9232 to 0.9578 and decreases the MAE from 0.01754 to 0.01617.

(a)



(b)



(c)

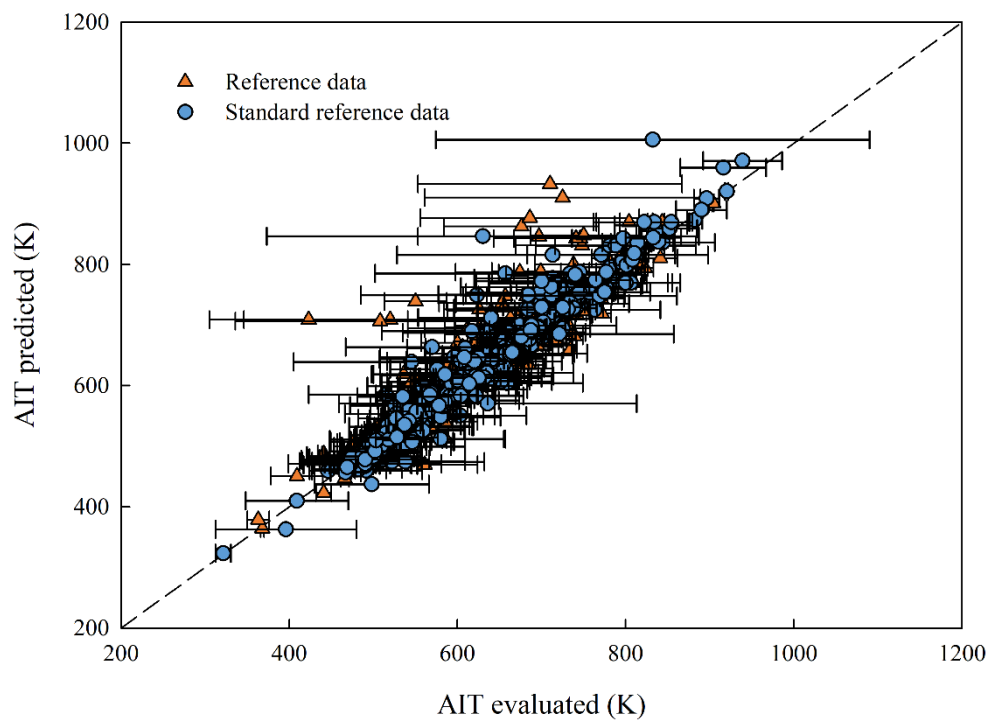
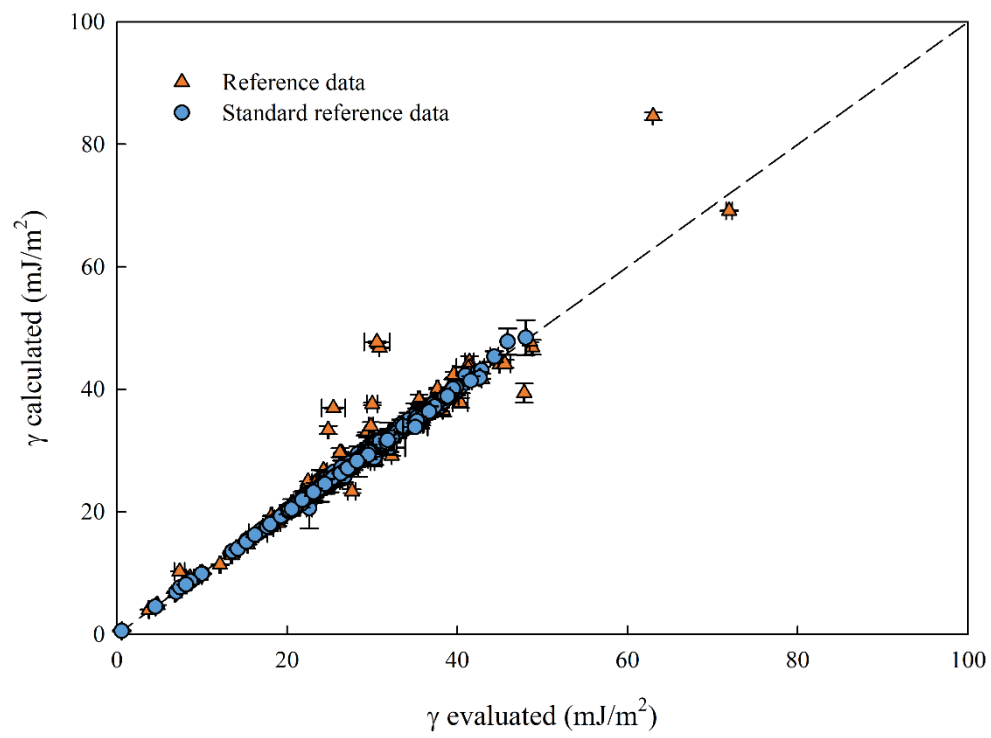
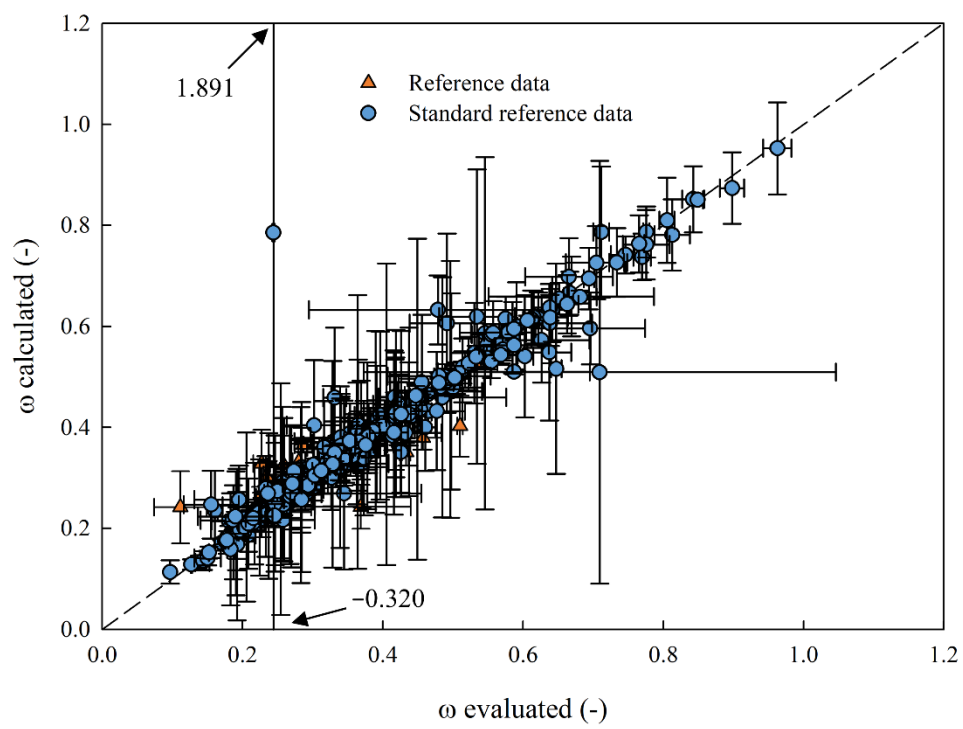


Fig. 2 Comparison of evaluated thermophysical property values with model predictions for the three fixed properties: (a) flash point (FP), (b) octanol–water partition coefficient ($\log K_{ow}$), and (c) autoignition temperature (AIT)

(a)



(b)



(c)

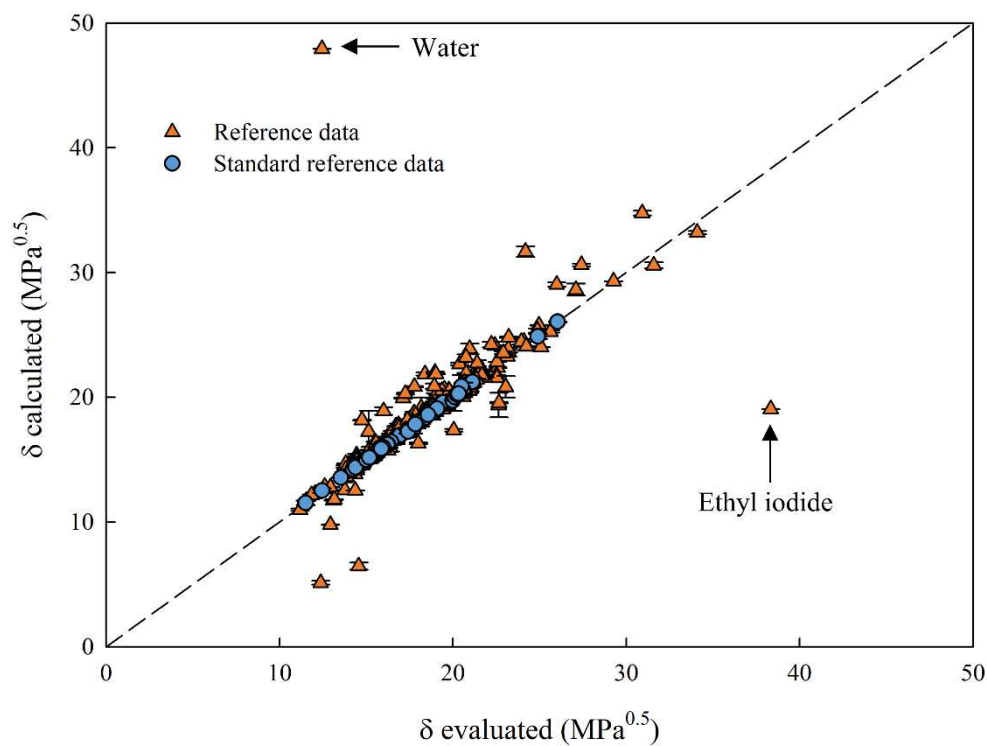


Fig. 3 Comparison of evaluated thermophysical property values with propagated estimates for the three derived properties: (a) surface tension (γ), (b) acentric factor (ω), and (c) Hildebrand solubility parameter (δ). The error bar exceeding the plotting range is truncated for visualization

Table 5 Agreement between comparison values and evaluated data, standard reference data, and reference data, estimated using mean absolute error (MAE) and coefficient of determination (R^2)

Property	Evaluated data		Standard reference data		Reference data	
	MAE	R^2	MAE	R^2	MAE	R^2
Flash point (FP)	10.08 K	0.9228	7.124 K	0.9555	19.10 K	0.8321
Octanol–water partition coefficient ($\log K_{ow}$)	0.2137	0.9579	0.1372	0.9776	0.3195	0.9388
Autoignition temperature (AIT)	24.12 K	0.8834	17.92 K	0.9393	34.99 K	0.7962
Surface tension (γ)	0.6225 mJ/m ²	0.9500	0.2100 mJ/m ²	0.9976	1.577 mJ/m ²	0.9041
Acentric factor (ω)	0.01764	0.9261	0.01754	0.9232	0.02003	0.9747
Hildebrand solubility parameter (δ)	0.6694 MPa ^{0.5}	0.6365	0.04137 MPa ^{0.5}	0.9990	0.8050 MPa ^{0.5}	0.6055

3.3. Characteristics and Utility of the Dataset

Traceability (Criterion 4, Section 2.4) was addressed separately for fixed and derived properties to account for differences in their data sources. For fixed properties (FP, $\log K_{ow}$, and AIT), each value was linked to the original peer-reviewed literature, ensuring that every evaluated entry could be traced to specific experimental measurements. For derived properties (γ , ω , and δ), traceability was based on the underlying properties used in the propagation relations. Critical temperature and pressure are taken from the original KDB dataset [58]. Enthalpy of vaporization, liquid density, and correlation coefficients for vapor pressure and surface tension were sourced from DIPPR [10] and NIST-TDE [13], with Acree's compilations [61, 62] used as needed. These databases document their evaluation procedures, providing a clear provenance chain. Instead of linking a derived property value directly to a single experimental publication, each value is associated with an evaluated correlation that has independently established provenance.

Each evaluated data entry includes not only the property value but also metadata such as expanded uncertainty, quality classification (reference data or standard reference data), and the number of experimental data points supporting the evaluation. These metadata allow users to distinguish standard reference data from reference data that do not meet all registration criteria but remain scientifically useful. The inclusion of documented evaluation records and metadata supports the reliability of each evaluated data entry. Although the KDB platform applies a five-level classification system as described in the general KDB framework [17], this study uses a simplified two-level classification, which is sufficient for the evaluation and cross-checking results presented here.

All evaluated data are available through the KDB platform (<https://www.mdlnkdb.com>), where users can access both the evaluated values and their associated metadata. The platform

supports searches by CAS Registry Number, IUPAC or common chemical names, SMILES, and InChI identifiers, and provides a structure-drawing interface for SMILES generation. For each registered compound, the property value, expanded uncertainty, quality classification, and number of supporting experimental data points are presented. A representative sample of the original references underlying the registered values is provided as Supplementary Information. The complete list may be exposed through the KDB web interface in a future release.

The resulting dataset contains representative thermophysical property values, with associated uncertainty estimates and quality classifications based on the evaluation framework. This structure allows users to select data according to the reliability requirements of specific applications, distinguishing standard reference data from broader reference data. The dataset provides a well-documented resource for applications that require reliable thermophysical property data and supports future data-driven studies by explicitly representing data quality. This framework is implemented as the operational evaluation protocol of the KDB platform, enabling continuous registration of newly collected literature data.

The proposed framework establishes a systematic procedure for constructing standard reference data, but several limitations should be noted. When reported uncertainties are not available, the procedure assigns a representative uncertainty based on the mean uncertainty of other data points for the same property. This approach may not accurately capture the true measurement uncertainty. The cross-check for fixed properties uses predictive models trained on datasets that can partially overlap with the current compilation, thereby limiting the independence of this validation step. For γ and ω , the comparison with propagated estimates assumes the correlation coefficients A – E are exact, leading to an underestimation of their associated uncertainties. In addition, the uncertainties of the critical constants from the original KDB dataset are sometimes very large, which reduces the effectiveness of the overlap criterion.

4. Conclusion

A systematic framework for constructing standard reference data was established and applied to six thermophysical properties: flash point, octanol–water partition coefficient, autoignition temperature, surface tension, acentric factor, and Hildebrand solubility parameter. The framework integrates literature collection, uncertainty evaluation, cross-checking with independent comparison methods, expert committee review, and traceability assessment to generate property values with quantified confidence.

Application of this framework to 82,488 raw literature data points yielded 2,363 registered standard reference data entries. Each entry includes its expanded uncertainty and quality classification, allowing users to assess both the property value and the associated confidence level. The cross-checking procedure supported registration decisions and identified inconsistencies in supporting database entries, thereby improving dataset quality. These results demonstrate the utility of the cross-checking procedure as both an evaluation criterion and a quality-assurance tool.

The evaluated data have been incorporated into the KDB platform and are publicly accessible with their associated metadata. Preservation of uncertainty, quality classification, and evaluation outcomes alongside property values ensures that the resulting dataset is a reliable resource for scientific and engineering applications that require thermophysical property data.

In summary, this work formalizes and validates a traceable, uncertainty-aware evaluation framework for six thermophysical properties. The results indicate that a systematic evaluation workflow can consistently convert heterogeneous literature data into reliable standard reference data within the KDB framework. Future work will extend the framework to additional properties and further automate the evaluation workflow within the KDB framework.

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