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# Aqueous Henry's Law Constants, Infinite Dilution Activity Coefficients, and Water Solubility: Critically Evaluated Database, Experimental Analysis, and Prediction Methods

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A dissertation submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

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# ABSTRACT

## Aqueous Henry's Law Constants, Infinite Dilution Activity Coefficients, and Water Solubility: Critically Evaluated Database, Experimental Analysis, and Prediction Methods

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A database containing Henry's law constants, infinite dilution activity coefficients and solubility data of industrially important chemicals in aqueous systems has been compiled. These properties are important in predicting the fate and transport of chemicals in the environment. The structure of this database is compatible with the existing DIPPR® 801 database and DIADEM interface, and the compounds included are a subset of the compounds found in the DIPPR® 801 database. Thermodynamic relationships, chemical family trends, and predicted values were carefully considered when designating recommended values.

Henry's law constants and infinite dilution activity coefficients were measured for toluene, 1-butanol, anisole, 1,2-difluorobenzene, 4-bromotoluene, 1,2,3-trichlorobenzene, and 2,4-dichlorotoluene in water using the inert gas stripping method at ambient pressure (approximately 12.5 psia) and at temperatures between 8°C and 50°C. Fugacity ratios, required to determine infinite dilution activity coefficients for the solid solutes, were calculated from literature values for the heat of fusion and the liquid and solid heat capacities. Chemicals were chosen based on missing or conflicting data from the literature.

A first-order temperature-dependent group contribution method was developed to predict Henry's law constants of hydrocarbons, alcohols, ketones, and formats where none of the functional groups are attached directly to a benzene ring. Efforts to expand this method to include ester and ether groups were unsuccessful. Second-order groups were developed at a reference condition of 298.15 K and 100 kPa. A second-order temperature-dependent group contribution method was then developed for hydrocarbons, ketones, esters, ethers, and alcohols. These methods were compared to existing literature prediction methods.

Keywords: DIPPR, database, Henry's law constant, water solubility, infinite dilution activity coefficient

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# 1 Introduction

A growing global concern is the fate and transport of chemicals in the environment in addition to health and safety risks associated with chemical exposure. The Toxic Substances Control Act (TSCA) was passed in 1976 in the United States, and it requires the U.S. Environmental Protection Agency (EPA) to estimate risks of chemicals prior to commercialization [1]. The EPA has developed a process to estimate risks associated with a chemical to ensure it will not pose an unreasonable risk if commercialized. Properties used in these risk assessments include water solubility, octanol/water partition coefficients, and Henry's law constants. The Registration, Evaluation and Authorization of Chemicals (REACH) is a new policy concerning chemical regulations in Europe that became effective June 2007 throughout the European Union [2]. REACH requires industry to provide health, safety, and environmental information that will aid in the management of risks. Properties required by REACH include water solubility and the octanol/water partition coefficient [3, 4].

It is estimated that experimental values are available for less than 1% of the approximately 84,000 compounds included in TSCA and the 100,000 compounds included in REACH [5]. This means that environmental regulations rely heavily on prediction methods. A prediction method is only as good as the data used to develop the method. Prediction methods developed using evaluated data allow for superior prediction method development performance.

DIPPR® Projects 911 and 912 were initiated in 1991 by AIChE/DIPPR® with the goal of compiling data and prediction methods for important environmental, safety, and health properties of chemicals that are regulated and important in industry [6]. The information was compiled as the Environmental and Safety Properties (ESP) database. In November 2009, the DIPPR® 801 steering committee decided that a thorough review should be conducted on select compounds in order to evaluate the status of the DIPPR® ESP database. As a result of the review, it was decided to build a new database (801E) focusing on select properties. The properties of primary interest are aqueous Henry's law constant ($k_H$), infinite dilution activity coefficient of a chemical in water ($\gamma_i^\infty$), and the solubility of a compound in water ($x_i^{aq}$). The infinite dilution activity coefficient of water in the chemical, the solubility of water in a chemical, and the octanol/water partition coefficients were included when available. However, these properties were given low priority meaning they were not reviewed as thoroughly due to time constraints and lower interest from the DIPPR® steering committee. An overview of the properties included in the 801E database is given in Chapter 2.

The first objective of this project was to compile a database containing primary, experimental data for $k_H$, $\gamma_i^\infty$, and $x_i^{aq}$ for 500 compounds. An overview of the database is given in Chapter 3. Accepted values were designated for $k_H$, $\gamma_i^\infty$, and $x_i^{aq}$ by evaluating the available literature data. Recommendations were given for values at a single temperature or over a temperature range depending on the amount of available literature data. The data evaluation process is described in Chapter 4. The second objective was to perform temperature-dependent measurements of $k_H$ and $\gamma_i^\infty$ for seven compounds to fill in data gaps and provide clarification for inconsistencies with reported experimental values. The experimental methods and results are given in Chapters 5 and 6. The third objective was to analyze and refine $k_H$ prediction methods using the evaluated database which is described in Chapter 7.

# 2 Overview of Properties

## 2.1 Definitions and Uses

### 2.1.1 Solubility of a Compound in Water

Water solubility ($x_i^{aq}$) is the maximum amount of a substance (gas, liquid, or solid) that will dissolve in a specified amount of water at a defined temperature and pressure [1]. This is an important property for predicting a chemical's environmental fate and its effects on biological systems. Highly water-soluble chemicals absorb easily into biological systems and typically degrade readily in the environment. However, highly water-soluble chemicals do not easily adsorb on soils and sediments or bioaccumulate. Solubility is a function of temperature, but it is often treated as a constant over environmental temperature ranges [7]. Generally, solubility increases with increasing temperature [8]. Other factors that affect solubility include pressure, pH, and the presence of additional chemical species [9-11]. In this project, the focus is $x_i^{aq}$ data of a single solute in pure water measured at temperatures below 373 K at or near atmospheric pressure. However, high-temperature data have been included for some compounds.

Some systems exhibit upper and/or lower critical solution temperatures. At temperatures below or above the lower or upper critical solution temperatures, respectively, the compound and water are completely soluble in each other resulting in one liquid phase. Compounds that have critical solution temperatures within the temperature limits of this study are noted in the database. In some studies reporting solubility data for solid compounds, compositions are reported for multiple portions of the phase diagrams (i.e. ice compositions). These other phase data are input (or mentioned) in the database. However, only data that meet the definition above of $x_i^{aq}$ for liquid water were analyzed in this study.

### 2.1.2 Solubility of Water in a Compound

The solubility of water in a compound is defined as the maximum amount of water that will dissolve in a given amount of compound at a specified temperature and pressure. This property is often measured in conjunction with $x_i^{aq}$ ($x_i^{aq}$ and the solubility of water in a compound are reported as mutual solubility values). Recommended values were not provided in this study because this is a low priority property, so a thorough literature review was not conducted for this property. This property is not as important as other properties when determining the environmental fate of hydrophobic compounds. However, data were briefly examined during the data analysis portion of this project. This is discussed in more detail in Section 4.1.

### 2.1.3 Henry's Law Constant

In environmental impact studies, Henry's law constants ($k_H$s) are used to determine the fate and transport of chemicals in air and water by determining volatilization or absorption tendencies [12, 13]. Chemicals with higher $k_H$s partition towards air while chemicals with lower $k_H$s partition towards water [1]. Additional uses of $k_H$ values include the design and optimization of air-stripping columns that remove contaminants from groundwater as well as applications in the pharmaceutical and food science industries [14].

The definition of $k_H$ is given by

$$k_H \equiv \lim_{x_i \to 0} \frac{\hat{f}_i^L}{x_i}, \qquad 2.1$$

where $\hat{f}_i^L$ is the partial fugacity of compound $i$ in solution, and $x_i$ is the mole fraction in the liquid phase [15-17]. This definition is applicable at all temperatures and pressures [16]. Application of l'Hôpital's rule equates $k_H$ to the slope of the tangent line of the $\hat{f}_i^L$ versus $x_i$ curve at $x_i = 0$. The equation of this tangent line produces Henry's law:

$$\hat{f}_i^L = x_i k_H . \qquad 2.2$$

Most systems are represented by Henry's law for small values of $x_i$. The concentration at which system behavior deviates from Henry's law varies with every system, although an upper concentration of 0.01 mole fraction has been recommended [18, 19]. An activity coefficient can be added to correct for non-idealities caused by higher concentrations. Corrections can also be introduced for systems at high pressures. If ideal gas behavior is assumed, Equation 2.2 simplifies to

$$y_i P = x_i k_H , \qquad 2.3$$

where $y_i$ is the mole fraction in the vapor phase and $P$ is the total pressure. In this study, $k_H$ refers to aqueous systems.

The Gibbs energy of hydration, $\Delta G_{hyd}^{\infty}$, is defined as the process of transferring a molecule from an ideal gas at a reference pressure to a hypothetical infinitely dilute solution with a solute mole fraction of unity[20-22]. A relationship between $k_H$ and $\Delta G_{hyd}^{\infty}$ is

$$RT\ln\left(\frac{k_H}{P_{ref}}\right) = \Delta G_{hyd}^{\infty}, \qquad 2.4$$

where $P_{ref}$ is 100 kPa. Unit conversions may need to be included in Equation 2.4 depending on the units of the reference state. Temperature and pressure derivatives link $\Delta G_{hyd}^{\infty}$ to additional properties often referred to as derivative properties. These derivative properties are the enthalpy of hydration ($\Delta H_{hyd}^{\infty}$), heat capacity of hydration ($\Delta Cp_{hyd}^{\infty}$), and partial molar volume ($V^{\infty}$) at infinite dilution:

$$RT^2\left(\frac{\partial \ln k_H}{\partial T}\right)_P = -\Delta H_{hyd}^{\infty}, \qquad 2.5$$

$$\left(\frac{\partial}{\partial T}\left[RT^2\frac{\partial \ln k_H}{\partial T}\right]\right)_P = -\Delta Cp_{hyd}^{\infty}, \qquad 2.6$$

$$RT\left(\frac{\partial \ln k_H}{\partial P}\right)_T = V^{\infty}. \qquad 2.7$$

Data for derivative properties were not included in this study. These relationships are mentioned because they are used in some prediction methods (discussed in Chapter 7).

Values of $k_H$ first increase with temperature, reach a maximum typically between 373 and 473 K, and then decrease with temperature [22]. Most compounds do not have enough reported temperature-dependent data to see this whole trend. There are several different reported units for

$k_H$. Units include the ratio of partial pressure ($P_i$) and solute concentration in a dilute solution, $P_i/x_i$ or $P_i/C_i^L$, where $C_i^L$ is the concentration, in units such as moles per liter, in the liquid phase. The aqueous $k_H$ is also reported as a ratio of the air and water concentrations making it unitless—either $y_i/x_i$ or $C_i^{air}/C_i^L$ where $C_i^{air}$ is the concentration in the vapor phase. While both of these ratios are unitless, their numerical values can differ significantly [23]. A universal conversion between the various ratios is done assuming the vapor phase behaves as an ideal gas and that the solution is pure water. These assumptions are valid under environmental conditions.

The air-water partition coefficient is the mole fraction ratio of the solute in air to that in water, and by definition it is not limited by the requirement of infinite dilution. In the environmental field, it is often used synonymously with $k_H$ despite different thermodynamic definitions [17, 24-26]. The conversion between the air-water partition coefficient and $k_H$ is straightforward for dilute solutions at environmental conditions which is why the terms are often used synonymously. The conversion becomes more complex at high temperatures and pressures. In the database, any reported $k_H$s or air-water partition coefficients that are measured for environmental purposes were treated as experimental $k_H$s.

The $k_H$ values measured for compounds that hydrate or dissociate in water are typically apparent $k_H$ values. Hydration or dissociation can be accounted for in order to calculate an intrinsic $k_H$ [23, 27]. No efforts were made to account for dissociation or hydration in this study. It is assumed that literature $k_H$ values are apparent $k_H$ values unless otherwise noted. In this study, $k_H$ data for strong electrolytes were typically left unevaluated due to the spread in data partially caused by the variety of pH conditions reported in the literature.

### 2.1.4 Infinite Dilution Activity Coefficients: Chemical in Water

Activity coefficients are an indicator of the nonideal behavior of a mixture. The activity coefficient of species *i* ($\gamma_i$) is defined as

$$\gamma_i \equiv \frac{\hat{f}_i}{x_i f_i^L} \qquad 2.8$$

where $\hat{f}_i$ is the partial fugacity of compound *i* in solution, $f_i^L$ is the pure liquid fugacity of species *i*, and $x_i$ is the mole fraction in the liquid phase. The infinite dilution activity coefficient ($\gamma_i^\infty$) is the limiting value as $x_i$ goes to zero. In this discussion, $\gamma_i^\infty$ specifically refers to systems in which the solvent is water.

Thermodynamic relationships exist between $\gamma_i^\infty$ and $x_i^{aq}$, $k_H$ and the octanol-water partition coefficient [28]. Relationships between $\gamma_i^\infty$, $x_i^{aq}$, and $k_H$ are given in Section 4.1. Environmental applications of $\gamma_i^\infty$s include assessments of aquatic toxicity, leaching, soil and sediment transport properties, sorption, bioconcentration, and volatilization [29]. Other applications include modeling evaporation rates [12], choosing the most selective solvent for extraction [30], and developing constants in empirical equations for excess functions which are then used to predict fluid phase equilibrium.

### 2.1.5 Infinite Dilution Activity Coefficients: Water in Chemical

The discussion for $\gamma_i^\infty$ applies here for the infinite dilution activity coefficient of water in a chemical, but the difference is that water is the solute and the chemical is the solvent. This property has low priority in this study because it is uncommon in environmental applications. Thorough literature and data analysis reviews have not been conducted in this study.

### 2.1.6 Octanol/Water Partition Coefficient

The octanol/water partition coefficient (KOW) is the equilibrium ratio of the concentrations of a chemical substance in *n*-octanol to that in water [1]. It is dimensionless and is often expressed as the base 10 logarithm. It can be used to predict the distribution of a chemical in living organisms (because octanol has a similar carbon to oxygen ratio as is found in lipid materials in animals [31]) or in the environment. For almost all non-ionic organic substances, KOW can be used to estimate other properties such as $x_i^{aq}$, soil/sediment absorption, biological absorption, bioaccumulation, and toxicity [1]. This property is temperature dependent [32]. KOW is a low priority property in this study since there are existing databases of KOW values [33, 34]. Data have been input when included in articles containing high priority properties. However, thorough literature and data analysis reviews have not been conducted.

## 2.2 Experimental Techniques

There are a variety of experimental methods that have been reported to measure the properties included in this study. Many of the methods can be used to obtain more than one property due to the relationships between properties (discussed in Section 4.1).

### 2.2.1 Solubilities

The methods to measure solubilities in which the solvent is a liquid are similar for all solute-solvent combinations. The solubility of water in a compound and $x_i^{aq}$ are often measured in the same study and reported as mutual solubility data. Many solubility methods consist of equilibrating water with excess compound and analyzing the composition of one or both of the resulting phases. There are a variety of equilibration and analytical techniques employed in the literature to accomplish this. The experimental methods are applicable over limited solubility ranges due to adsorption and emulsion problems and detection limitations, so the solubility needs to be predicted in order to choose the correct testing method. The methods are discussed in further detail in Appendix A.

### 2.2.2 Henry's Law Constants

Static or dynamic equilibration techniques can be used to measure $k_H$. Static equilibration involves the direct measurement of the air and/or water concentrations in a closed, equilibrated system. Methods include single equilibration, multiple equilibration, equilibrium partitioning in closed systems (EPICS), and variable headspace techniques. Static equilibration techniques are usually only done for higher concentrations due to the difficulty in measuring low concentrations in both phases [19]. Dynamic equilibration involves some type of air/water exchange. Two methods of this type are inert gas stripping and concurrent flow. Experimental methods are discussed in more detail along with limitations in Appendix A.

### 2.2.3 Infinite Dilution Activity Coefficients

There is overlap between the methods used to measure $k_H$ and $\gamma_i^\infty$ due to the thermodynamic relationship between these two properties (see Section 4.1). Many papers report both properties from the same experimental data. Often multiple techniques are required to measure values over a range of temperatures due to measurement limitations. It is ideal to apply more than one measurement technique to ensure consistency in results [35]. Experimental methods are discussed in more detail along with limitations in Appendix A.

### 2.2.4 Octanol/Water Partition Coefficients

The methods used to measure KOWs are similar to some of the methods used to measure $x_i^{aq}$. These methods include equilibrating a compound with 1-octanol and water and determining the concentration using an analytical technique. Another common method involves estimating the KOW based on gas chromatography (GC) retention data of the compound and reference compounds. Each method covers a range of values, so KOW should be predicted in order to determine the proper testing technique. Experimental methods are discussed in more detail along with limitations in Appendix A.

# 3 Database Overview

## 3.1 Background

It was decided at the May 2010 DIPPR® meeting by BYU staff and DIPPR® sponsors to build a new database containing the properties outlined in Chapter 2 because more work would be involved in fixing the ESP database than in starting fresh. In the original ESP database, data for the properties outlined in Chapter 2 were only included at 298.15 K, and the properties were included in the constant values tables. It was decided to include temperature-dependent data in addition to the constant values (defined at 298.15 K) in the new database. Due to the notation allowed in Microsoft Access®, the properties had to be represented by letter abbreviations instead of symbols. Separate abbreviations were required for the constant value and temperature-dependent properties. The abbreviations are given in Table 3.1. The symbols $k_H$, $x_i^{aq}$, and $\gamma_i^\infty$ will continue to be used throughout this document in the text and plots because they are more intuitive.

Table 3.1: Abbreviations used in 801E database

| Property | Constant Value | Temperature-Dependent |
|---|---|---|
| Infinite dilution activity coefficient of compound in water | ACCW | ACCWT |
| Infinite dilution activity coefficient of water in compound | ACWC | ACWCT |
| Aqueous Henry's law constant | HLC | HLCT |
| Octanol/water partition coefficient | KOW | KOWT |
| Solubility of compound in water | SOLC | SOLCT |
| Solubility of water in a compound | SOLW | SOLWT |

### 3.2 Database Structure and Data Entry

This new database, DIPPR® 801E, has a similar format to the 801 database so that it is compatible with DIADEM, the DIPPR® 801 software interface. In order to make the process of data entry easier while reducing the opportunities for entry error, DIADEM was modified slightly. Units were added so that they can be selected from dropdown menus. Due to assumptions in the unit conversions, two columns were added to the database so that it stores the original values and units in the database after the data for each property are converted to the default unit. There is not a way to view these original values or perform more complex unit conversions using DIADEM, but a future user of the database could look up the original value and perform a more exact unit conversion if desired.

Data were considered constant values or temperature-dependent. The constant values properties are defined at 298.15 K and 1 atm. Experimental values within ±5 degrees of 298.15 K were included in the constant values table. The actual temperature and pressure were included in a note if they differed from 298.15 K or 1 atm, respectively. All values at 298.15 K were also input as temperature-dependent data in addition to data at other temperatures. There were instances when articles included measurements for some chemicals only at temperatures outside of the constant value range. In these instances, the data were only entered in the temperature-dependent table. If data of non-dissociating compounds were reported as a function of pH, only the values at pH ≈ 7 were analyzed. When data were input, they were labeled as “Unevaluated”. As datasets were evaluated, the label was changed to “Accepted”, “Not Used”, or “Rejected” based on the quality of the dataset. These categories allow a future user to know which data were considered during the evaluation process.

At the conclusion of this project, recommended ("Accepted") values have been determined for at least one property for 509 compounds. There are entries for over 800 compounds due to the data entry process; however, not all of the data have been evaluated. Data were entered by reference, and all data for any DIPPR® 801 chemical mentioned in a reference were included. Table 3.2 summarizes the number of data points that have been considered during evaluation and the number of compounds with recommended values for each property. Due to the lack of reliable data, not all of the high priority properties were analyzed for each compound which is why each property has a different number of compounds with recommendations. Based on the availability of temperature-dependent data, some compounds have recommendations for a temperature range while other compounds only have recommendations for a single temperature (typically 298.15 K). Table 3.3 summarizes the total number of evaluated compounds per chemical family. The entry numbers given in Table 3.2 reflect the actual entries retrieved directly from the literature. They do not include the derived entries that were added during the data evaluation process of this study (i.e. $k_H$ values derived from $x_i^{aq}$ data, etc.). The compound totals include the American Petroleum Institute (API) recommendations that were accepted in this study (discussed in Section 4.5). The data evaluation process is discussed in detail in Chapter 4.

Table 3.2: Summary of 801E entries

| Property | Evaluated Data Points | Compounds with Recommendations |
|---|---|---|
| $\gamma_i^\infty$ | 1350 | 407 |
| $k_H$ | 3950 | 445 |
| $x_i^{aq}$ | 7617 | 481 |
| Overall | 12917 | 509 |

Table 3.3: Summary of the number of evaluated compounds (#) per chemical family

| Family | # | Family | # | Family | # |
|---|---|---|---|---|---|
| 1-Alkenes | 14 | Dialkenes | 2 | Other Alkanes | 2 |
| 2,3,4-Alkenes | 4 | Dicarboxylic Acids | 3 | Other Alkylbenzenes | 10 |
| Acetates | 17 | Dimethylalkanes | 7 | Other Amines, Imines | 7 |
| Aldehydes | 19 | Diphenyl/Polyaromatics | 1 | Other Condensed Rings | 11 |
| Aliphatic Ethers | 13 | Elements | 6 | Other Ethers/Diethers | 7 |
| Alkylcyclohexanes | 4 | Epoxides | 6 | Other Inorganics | 1 |
| Alkylcyclopentanes | 1 | Formates | 7 | Other Monoaromatics | 1 |
| Alkynes | 8 | Inorganic Bases | 1 | Other Polyfunctional C, H, O | 6 |
| Aromatic Alcohols | 14 | Inorganic Gases | 5 | Other Polyfunctional Organics | 2 |
| Aromatic Amines | 16 | Ketones | 26 | Other Saturated Aliphatic Esters | 6 |
| Aromatic Carboxylic Acids | 4 | Mercaptans | 5 | Peroxides | 2 |
| Aromatic Chlorides | 11 | Methylalkanes | 8 | Polyfunctional Acids | 1 |
| Aromatic Esters | 9 | Methylalkenes | 2 | Polyfunctional Amides/Amines | 7 |
| C, H, Br Compounds | 14 | *n*-Alcohols | 18 | Polyfunctional C, H, N, Halide, (O) | 2 |
| C, H, F Compounds | 8 | *n*-Aliphatic Primary Amines | 8 | Polyfunctional C, H, O, Halide | 6 |
| C, H, I Compounds | 7 | *n*-Alkanes | 14 | Polyfunctional C, H, O, N | 3 |
| C, H, Multihalogen Compounds | 3 | *n*-Alkylbenzenes | 11 | Polyfunctional C, H, O, S | 1 |
| C, H, $NO_2$ Compounds | 17 | Naphthalenes | 4 | Polyfunctional Esters | 4 |
| C1/C2 Aliphatic Chlorides | 19 | Nitriles | 12 | Polyols | 3 |
| C3 & Higher Aliphatic Chlorides | 11 | Nitroamines | 3 | Propionates and Butyrates | 13 |
| Cycloaliphatic Alcohols | 1 | Organic Salts | 2 | Sulfides/Thiophenes | 6 |
| Cycloalkanes | 5 | Other Aliphatic Alcohols | 21 | Unsaturated Aliphatic Esters | 4 |
| Cycloalkenes | 4 | Other Aliphatic Amines | 9 | | |

Data were entered with the original values and units to avoid any errors from external conversions. The only exceptions were when articles only report data as plots or regressions of experimental values. *DataThief* [36] was used to extract values from plots of experimental data. When authors only reported temperature-dependent correlations of their experimental data, the correlations were used to calculate values at the measurement temperatures reported by the authors. These values were classified as “Smoothed” in the database. Some authors report multiple values at the same temperature. The average of these values was input in order to not give extra weight to the dataset during analysis.

The focus of this database was on primary, experimental data. Due to time constraints, an additional focus was on post 1950 English references. It was assumed that more recent data are generally of higher quality than older data due to improvements in analytical techniques and higher material purities. Many of the older and/or foreign articles were not readily available, and the foreign articles required translating. Due to time constraints, it was not realistic for all of these types of articles to be included. Data from these articles were selectively input based on the availability of data from more recent English references. Data found in handbooks would be interesting to include in the database to compare with primary data, but these references were also excluded due to ambiguities and the time required for data entry. The original sources of handbook data (experimental versus predicted) are often excluded or unclear making it difficult to determine the reliability of the reported values.

Guidelines were developed that aided in data classification. These guidelines explain how to label data (i.e., classifying data as “experimental” or “predicted”). Issues that were encountered during the data entry process were clarified to establish consistency in the database. The guidelines also include assumptions and limitations for the various measurement techniques which was useful during the data analysis process.

## 3.3 Unit Conversions

In order to compare values from different references, all literature values needed to be converted to the same units. The unit conversions for the temperature-dependent properties accounted for the temperature-dependence of the conversion. For example, some $x_i^{aq}$ and $k_H$ conversions required liquid densities. When the temperature-dependent data were converted, the liquid densities at the correct temperature were used. There were additional assumptions with some of the unit conversions. These assumptions in addition to the default units are listed in Table 3.4. The assumptions for the $k_H$ unit conversions are valid since the data included in the database were typically measured at atmospheric pressure using dilute solutions. Many of the solubility data were reported in units that did not require any assumptions in order to perform the conversion to the default unit. When assumptions were required, it was assumed that volumes were additive. This assumption was generally only needed for compounds with small solubilities. Any volume changes due to non-ideality would be negligible. Initially only liquid or theoretical liquid densities were used for the solubility conversions. In some cases extrapolating the liquid density curve to temperatures where the compound is a solid led to obviously erroneous values (gave negative solubility values). Therefore, the volume of the liquid or solid solute was calculated using the liquid or solid densities, respectively, when using additive volumes for solubility conversions. If the solute was a gas, it was assumed that the added volume was negligible.

Table 3.4: Unit conversion assumptions

| Property | Unit Conversion Assumptions | Default Units |
|---|---|---|
| HLC | • Ideal gas with pressure of 1 atm<br>• Solution treated as pure water (since infinitely dilute) | kPa·mol/mol |
| SOLW/SOLC | • Additive volumes if solute is a solid or liquid<br>• Solution considered pure solvent if solute is gas<br>• Solution considered pure solvent if solute is a solid that does not have a solid density equation (i.e. 1-heptadecanol)<br>• Conversions treated as per amount of solution (i.e. g/100g solution) unless authors state otherwise (i.e. g/100g H2O) | mol frac. |
| ACCW/ACWC | None | unitless |
| KOW | None | Log KOW |

# 4 Data Evaluation

Because of the thermodynamic relationships between $k_H$, $x_i^{aq}$, and $\gamma_i^{\infty}$, reported values of these different properties can be conveniently compared. In this study, the combined data from the three properties were often used to obtain temperature regressions and recommended values for each property. For compounds where the assumptions of the thermodynamic relationships were not met (meaning the data from all the properties could not be combined), these relationships still helped identify outliers in reported data making it easier to designate recommended values. Notes in the database indicate the data that were combined to obtain regressions for each compound and property. In addition, experimental factors, temperature-dependent trends, chemical family plots, and literature recommendations were also used to evaluate data. All of these are discussed in further detail.

## 4.1 Property Relationships

A relationship between $k_H$ and $x_i^{aq}$ is given by evaluating equation 2.3 at the solubility limit

$$k_H = \frac{P_i^{sat}}{x_i^{aq}} \qquad 4.1$$

where $P_i^{sat}$ is the vapor pressure of solute *i*. This relationship is valid for hydrophobic chemicals with $x_i^{aq}$ values below approximately 0.001 mole fraction. It assumes that the solubility of water in the compound (SOLC) is negligible so that the partial vapor pressure of solute is unaffected by the presence of water allowing it to be treated as $P_i^{sat}$ [12, 19, 23]. The assumptions break down when SOLC exceeds approximately 0.1 mole fraction. In addition, $x_i^{aq}$ and $P_i^{sat}$ must reference the same physical state [37]. In this study, a pressure of 101.325 kPa was assumed for gases in order to convert $k_H$ to $x_i^{aq}$ values and vice versa. For gases, $k_H$ and $x_i^{aq}$ are used interchangeably. In the literature, $k_H$ values calculated from Equation 4.1 are usually reported as experimental.

A relationship between $k_H$ and $\gamma_i^\infty$ is obtained by substituting the definition of $\gamma_i$ (Equation 2.8) into that of $k_H$ (Equation 2.1),

$$k_H = \gamma_i^\infty f_i^L , \qquad 4.2$$

where $f_i^L$ is the fugacity of pure species $i$ in the liquid phase, and $x_i$ is the mole fraction in the liquid phase. At atmospheric conditions for liquid solutes, this simplifies to:

$$k_H = \gamma_i^\infty P_i^{sat} . \qquad 4.3$$

This relationship is more thermodynamically rigorous than Equation 4.1. Combining Equations 4.1 and 4.3 yields a relationship between $\gamma_i^\infty$ and $x_i^{aq}$ for hydrophobic liquids:

$$\gamma_i^\infty = \frac{1}{x_i^{aq}} . \qquad 4.4$$

The same assumptions that make Equation 4.1 valid also apply for Equation 4.4. Equation 4.4 is valid for $\gamma_i^\infty$ values greater than 1000 [38]. When available, SOLC data were examined during the data analysis procedure to check the validity of Equations 4.1 and 4.4. It is possible to use both SOLC and $x_i^{aq}$ to obtain $\gamma_i^\infty$ when the assumptions of Equation 4.4 are violated [23, 39] . However, since SOLC data were not critically evaluated, $\gamma_i^\infty$ and $k_H$ values were not determined from $x_i^{aq}$ when SOLC was above approximately 0.1 mole fraction. All of the valid ranges of the thermodynamic relationships discussed in this section are approximate. The thermodynamic relationships were applied outside of these ranges if chemical and/or chemical family data indicated a different range of applicability.

When the solute is a solid or a gas, it is necessary to determine a hypothetical $f_i^L$ in order to relate $k_H$ and $\gamma_i^\infty$. For compounds that are solids at the specified temperature (so only the solid $P_i^{sat}$ is known), a fugacity ratio must be used to account for the difference in states. The fugacity ratio, Ψ, of species *i* is defined as the ratio of the solid and liquid fugacities at the system temperature, *T*, and pressure, *P*:

$$\Psi_i \equiv \frac{f_i^S(T,P)}{f_i^L(T,P)}. \tag{4.5}$$

Substituting Equation 4.5 into 4.2 yields

$$k_H = \gamma_i^\infty \frac{P_i^{sat}}{\Psi}, \tag{4.6}$$

which assumes that $f_i^S$ is equal to the solid $P_i^{sat}$. Combining Equations 4.1 and 4.6 provides a relationship between $\gamma_i^\infty$ and $x_i^{aq}$ for solids:

$$\gamma_i^\infty = \frac{\Psi}{x_i^{aq}}. \tag{4.7}$$

At the melting point ($Tm_i$), the solid and liquid fugacities are equal in both phases:

$$\frac{f_i^S(Tm_i,P)}{f_i^L(Tm_i,P)} = 1. \tag{4.8}$$

Multiplying Equation 4.5 by 4.8 leads to

$$\Psi_i = \frac{f_i^S(T,P)}{f_i^S(Tm_i,P)} \frac{f_i^L(Tm_i,P)}{f_i^L(T,P)}. \qquad 4.9$$

The residual Gibbs energy, $G_i^R$, is related to $f$ and $P$ by

$$G_i^R = RT \ln\left(\frac{f_i}{P}\right). \qquad 4.10$$

Rearranging Equation 4.10 and using partial derivatives leads to

$$\left(\frac{\partial \ln(f_i)}{\partial T}\right)_P = \left[\frac{\partial\left(G_i^R / RT\right)}{\partial T}\right]_P = -\frac{H_i^R}{RT^2} \qquad 4.11$$

where $H_i^R$ is the residual enthalpy. To integrate for a phase from $Tm$ to $T$ at constant $P$ gives

$$\frac{f_i(T,P)}{f_i(Tm_i,P)} = \exp \int_{Tm_i}^{T} -\frac{H_i^R}{RT^2} dT. \qquad 4.12$$

This is applied to both the solid and liquid ratios in Equation 4.9:

$$\Psi_i = \frac{\exp \int_{Tm_i}^{T} -\frac{H_i^{R,S}}{RT^2} dT}{\exp \int_{Tm_i}^{T} -\frac{H_i^{R,L}}{RT^2} dT} = \exp \int_{Tm_i}^{T} -\frac{\left(H_i^{R,S} - H_i^{R,L}\right)}{RT^2} dT. \qquad 4.13$$

Using the definition of residuals yields

$$-(H_i^{R,S} - H_i^{R,L}) = -\left[(H_i^S - H_i^{IG}) - (H_i^L - H_i^{IG})\right] = H_i^L - H_i^S \qquad 4.14$$

where $IG$ refers to the ideal gas property. The exact expression for $\Psi$ is

$$\Psi_i = \exp \int_{Tm_i}^{T} \frac{H_i^L - H_i^S}{RT^2} dT \,. \qquad 4.15$$

The temperature dependence of $H$ can be described using

$$H_i^L(T) - H_i^S(T) = \Delta H_{f,Tm} + \int_{Tm_i}^{T} Cp_i^L dT - \int_{Tm_i}^{T} Cp_i^S dT \qquad 4.16$$

where $\Delta H_{f,Tm}$ is the heat of fusion at the melting point and $Cp_i$ is the constant pressure heat capacity.

In the literature, the fugacity ratio is often approximated as

$$\Psi \cong \exp\left(\frac{\Delta H_{f,Tm}}{RT}\left(\frac{T}{Tm_i} - 1\right)\right) = \exp\left(\frac{\Delta S_{f,Tm}}{R}\left(1 - \frac{T}{Tm_i}\right)\right) \qquad 4.17$$

where $\Delta S_{f,Tm}$ is the entropy of fusion at the melting point [40, 41]. In many instances $\Delta S_{f,Tm}$ is estimated to be a constant value, 56.5 J/(mol·K), for all solid compounds. Van Noort found that using this estimated value for $\Delta S_{f,Tm}$ led to substantial random errors for some aromatic compounds [40].

In this study, Equations 4.15 and 4.16 were used with DIPPR® 801 property values to calculate Ψs. When $Cp_i$ data were not available, Equation 4.17 was used with DIPPR®801 $\Delta H_{f,Tm}$ values. The $Cp_i$ values in DIPPR® 801 are at saturation pressure above the normal boiling point (NBP). Below the NBP, saturated heat capacity and constant pressure heat capacity are used interchangeably. For most of the solid compounds included in this study, the temperature range of data did not extend beyond the NBP. Equation 4.16 requires $Cp_i^L$ values at temperatures below $Tm_i$ which cannot be measured. In order to use this equation, the DIPPR® 801 $Cp_i^L$ equations had to be extrapolated below $Tm_i$ which resulted in hypothetical values. The equation used for the error estimation of Ψ was determined using propagation of error, and the derivation is included in Appendix B. Fugacity Error Propagation. Many of the recommended solid $\gamma_i^\infty$ values from this study have high uncertainties due to the uncertainty in Ψ.

For compounds that are gases, estimating a hypothetical $f_i^L$ can be difficult for temperatures above the compound critical temperature [42]. Due to this difficulty, $\gamma_i^\infty$ values were not computed for any compound that is a gas at 1 atm and 298.15 K. This limit was chosen in order to simplify the data analysis process even though 298.15 K is not above the critical temperature for every gaseous compound. The total number of gaseous compounds analyzed in the database is small compared to compounds that are solids or liquids. Table 4.1 summarizes the number of compounds with recommended values (determined in this study) that are gases, liquids, or solids at 298.15 K and 1 atm. A summary of the property relationships used in this study is shown in Table 4.2 by the physical state of the solute.

Table 4.1: Number of compounds with recommended values per physical state at 298.15 K

| Phase at 298.15 K | Number of Compounds with Recommended Values |
|---|---|
| Gas | 39 |
| Liquid | 393 |
| Solid | 77 |

Table 4.2: Summary of property relationships used in this study

| | | | |
|---|---|---|---|
| Solid | $k_H = \frac{P_i^{sat}}{x_i^{aq}}$ | $k_H = \gamma_i^\infty \frac{P_i^{sat}}{\Psi}$ | $\gamma_i^\infty = \frac{\Psi}{x_i^{aq}}$ |
| Liquid | $k_H = \frac{P_i^{sat}}{x_i^{aq}}$ | $k_H = \gamma_i^\infty P_i^{sat}$ | $\gamma_i^\infty = \frac{1}{x_i^{aq}}$ |
| Gas | $k_H = \frac{101.325\ \text{kPa}}{x_i^{aq}}$ | - | - |

As was mentioned, $k_H$ and $\gamma_i^\infty$ were analyzed together and $x_i^{aq}$ analyzed separately for compounds where Equations 4.1and 4.4 are not valid. As an example, Figure 4.1 is a plot of $k_H$, $x_i^{aq}$, and $\gamma_i^\infty$ data for 2-methyl-1-butanol plotted as $\ln(k_H)$ versus inverse temperature. Literature $x_i^{aq}$ and $\gamma_i^\infty$ data were converted to $k_H$ using Equations 4.1 and 4.3. Although SOLC is significant (reported SOLC values range between 0.325-0.553 mole fraction over the temperature range of 293.15-303.15 K [43]), it is difficult to see a difference between the curves obtained from using only $k_H$ and $\gamma_i^\infty$ values and the curve that includes $x_i^{aq}$ data. The difference is more pronounced when all of the data are converted to $\ln(x_i^{aq})$ (Figure 4.2). Although all of the properties cannot be combined to obtain a regression, plotting the properties together aids in the data evaluation process because the data still follow similar temperature trends. This is especially useful when data for a property are only available from a single reference.

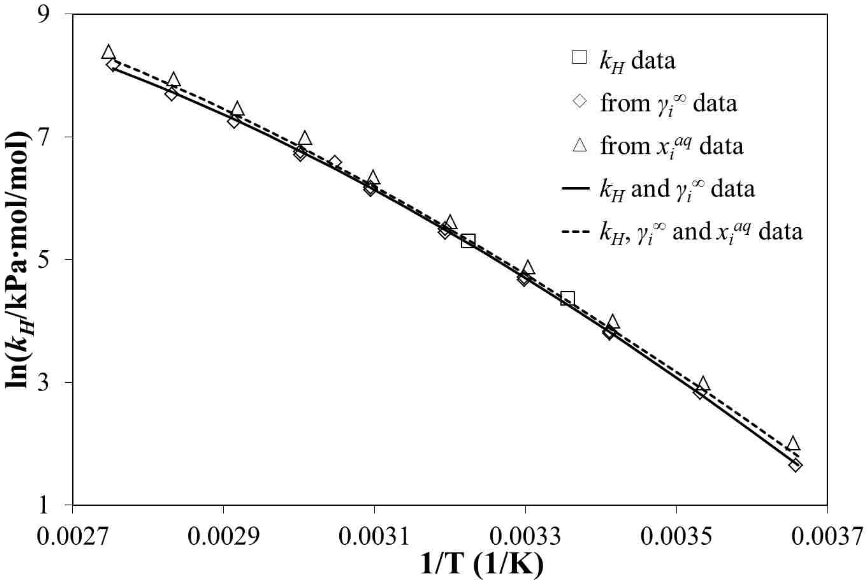

Figure 4.1: 2-Methyl-1-butanol $k_H$, $x_i^{aq}$, and $\gamma_i^\infty$ data plotted as $\ln(k_H)$ versus inverse temperature. References: [44-48]

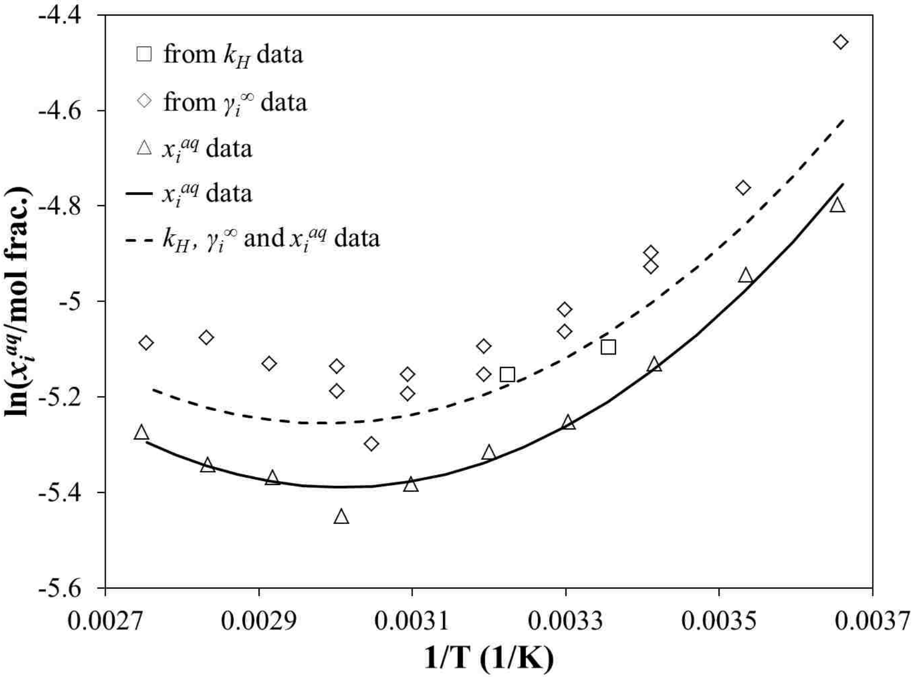

Figure 4.2: 2-Methyl-1-butanol $k_H$, $x_i^{aq}$, and $\gamma_i^\infty$ data plotted as ln($x_i^{aq}$) versus inverse temperature References: [44-48]

As was mentioned in Section 3.2, not all of the properties were analyzed for every compound. Some compounds did not have data for every property, and the assumptions used to relate the properties were not valid. For example, temperature-dependent $x_i^{aq}$ data were available for many aromatic alcohols but no literature $k_H$ or $\gamma_i^\infty$ data were found. Due to the high $x_i^{aq}$ and high SOLC, Equations 4.1 and 4.4 are not valid, so $k_H$ and $\gamma_i^\infty$ recommendations were not determined.

## 4.2 Experimental Factors

Experimental factors that were considered when choosing between conflicting datasets include accuracy of experimental method, reported chemical purity, reported experimental error, and agreement with other references. For example, adsorption problems have been noted for aqueous systems using the gas-liquid chromatography (GLC) method [49]. If GLC values are inconsistent with other values obtained using different methods, then the GLC dataset was rejected. In addition, if an author reported a dataset as having a large uncertainty and the dataset does not match up with other data, then the dataset with the high reported experimental error was rejected. Experimental limitations are included with experimental descriptions in Appendix B.

As an example, Figure 4.3 gives a plot of experimental $x_i^{aq}$ data for vanillin reported in the literature. The data from one of the references, d, does not match up with the data from the other references even though a reasonable experimental method was used with a low reported experimental uncertainty. Because the other references are consistent with each other, the data from reference d were rejected.

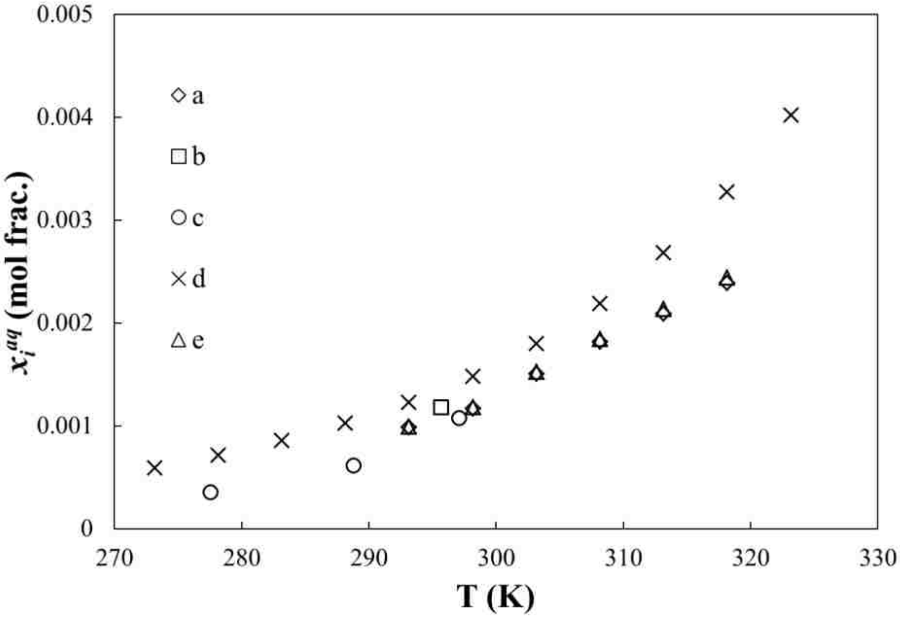

Figure 4.3: Literature $x_i^{aq}$ data for vanillin. References: a [50], b [51], c [52], d [53], e [54]

## 4.3 Temperature-Dependent Evaluation

When temperature-dependent data were available, correlations modeling the temperature-dependence of $k_H$, $x_i^{aq}$, and $\gamma_i^\infty$ were regressed. This section outlines a general procedure that was used to select the data that were suitable for the regressions. A Microsoft Excel® workbook was made to aid with data evaluation of these high priority properties. Temperature-dependent data were extracted from the database for an individual compound. A macro converted each of the values to $k_H$ and $\gamma_i^\infty$ using $P_i^{sat}$ from the DIPPR® 801 database. Plots were generated with all of the data to easily identify outliers. Any outliers were checked to ensure that the value was input correctly and that there was not a mistake with the unit conversion. At this stage, data were classified as "Accepted", "Rejected", or "Not Used". Criteria discussed in Sections 4.1and 4.2 were used to determine this data classification.

The data were then checked for "doubles". Some published papers report values for more than one property from the same experiment by using the property relationships discussed in Section 4.1. For example, $k_H$ and $\gamma_i^\infty$ values are both reported in some papers from the same experimental data. For a paper with both of these properties, converting $k_H$ values to $\gamma_i^\infty$ (or vice versa) would have given double weight to these values during data analysis since they were already reported as the other property. In addition, there are some instances where data have been doubly published. It was assumed that identical datasets reported by the same author in different papers are duplicates. Only one dataset of duplicate sets was included when determining regression coefficients, but both datasets were labeled as "Accepted". Once the doubles were identified, data were sorted to be input into a Mathcad® file. One last check was performed to ensure that all of the data points from the same dataset had the same classification. Datasets cannot have some points that are "Accepted" and others that are "Rejected". If there was a special case where there was a valid reason for rejecting some points from a dataset while accepting others (for example, the authors reported large errors at low temperatures), then the dataset had to be split into two separate datasets.

The classified data were then put into a template that was made using Mathcad®. Other input values required were pure-component properties available in DIPPR® 801. The user designated which data were to be used to determine recommended temperature-dependent regressions of all of the properties (i.e. $x_i^{aq}$, $k_H$, and $\gamma_i^{\infty}$ data were all included in the $k_H$ regression; only $k_H$ and $\gamma_i^{\infty}$ data were included in the $k_H$ regression; etc.).

The equations used to model temperature-dependence are given in Table 4.3 along with the corresponding DIPPR® equation numbers. DIPPR® Equations 5000 and 6000 were added specifically for this project for compounds with $x_i^{aq}$ data that do not conform to DIPPR® Equation 101.Various Mathcad® files were available that compared different regressions for compounds over the temperature range of the data. The equation comparisons available in the files are summarized in Table 4.4. The analyzer used F-test p-values to determine if regressed parameters were statistically significant (p-values $< 0.05$ indicated that an additional term was significant) when comparing equations that only differed by a single term. When comparing DIPPR® Equations 5000 and 6000 (case 3 for $\ln(x_i^{aq})$ in Table 4.4), the best equation was selected visually or based on $R^2$ values. Most of the compounds that deviate from DIPPR® Equation 101 have upper or lower critical solution temperatures within the temperature range of data in the database. These new equations are simple and generic resulting in a wide range of applicability. With all of the regressions, the best equation was used even if it did not fit the data perfectly. The equations are meant to be generic, so terms were not modified on a compound basis.

Table 4.3: DIPPR® 801 equation numbers

| DIPPR® Equation Number | Equation[a] |
|---|---|
| 101 | $\ln(Y) = A + \frac{B}{T} + C\ln(T) + DT^{E}$ |
| 5000 | $\ln(Y) = A + \frac{B}{T} + C\ln(T) + D \cdot \exp\left(\left\|1 - \frac{T}{E}\right\|\right)$ |
| 6000 | $\ln(Y) = A + \frac{B}{T} + C \cdot T + D\left(\left\|1 - \frac{T}{E}\right\|\right)^{1/3}$ |

[a] Y represents the property and A, B, C, D, and E are compound-specific coefficients

Table 4.4: Equation comparisons used in data analysis

| Property | Equation Comparisons |
|---|---|
| $\ln(k_H)$ & $\ln(\gamma_i^{\infty})$ | 1) $A + \frac{B}{T} + C\ln(T) + DT$ and $A + \frac{B}{T} + C\ln(T)$<br>2) $A + \frac{B}{T} + C\ln(T)$ and $A + \frac{B}{T}$ |
| $\ln(x_i^{aq})$ | 1) $A + \frac{B}{T} + C\ln(T) + \frac{D}{T^2}$ and $A + \frac{B}{T} + \frac{D}{T^2}$<br>2) $A + \frac{B}{T} + \frac{D}{T^2}$ and $A + \frac{B}{T}$<br>3) $A + \frac{B}{T} + C\ln(T) + D \cdot \exp\left(\left\|1 - \frac{T}{E}\right\|\right)$ and $A + \frac{B}{T} + C \cdot T + D\left(\left\|1 - \frac{T}{E}\right\|\right)^{1/3}$ |

The $\gamma_i^{\infty}$ regressions were derived from the $k_H$ regressions and not directly from the $\gamma_i^{\infty}$ data due to the scatter in $\gamma_i^{\infty}$ data. If the regressions were obtained directly from the $\gamma_i^{\infty}$ data, curvature often would not be significant due to the scatter in the data. In addition, compounds generally have more $k_H$ data than $\gamma_i^{\infty}$ data. The $\gamma_i^{\infty}$ regressions are derived from $k_H$ instead of $x_i^{aq}$ because the relationship between $\gamma_i^{\infty}$ and $k_H$ (Equation 4.3) is more thermodynamically rigorous than the relationship between $\gamma_i^{\infty}$ and $x_i^{aq}$ (Equation 4.4). For solid compounds, Ψs were used to convert the $k_H$ regressions to the $\gamma_i^{\infty}$ regressions. Since the $\gamma_i^{\infty}$ curves were derived from the $k_H$

regressions, there were really two $\gamma_i^\infty$ curves for every compound that had data above and below the melting point. For these compounds, a single curve was fit to the $\gamma_i^\infty$ values so that one equation covered the entire temperature range.

A temperature-dependent regression was classified as “Experimental” if experimental data from any of the properties were used and the property relationship assumptions discussed in Section 4.1 were valid. As was mentioned in Section 4.1, experimental SOLC values were checked when available. If SOLC values were significant at higher temperatures (> ~0.1 mole fraction), then only lower temperature $x_i^{aq}$ data were used to obtain the other properties. For example, with 3,5-xylenol, only $k_H$ and $\gamma_i^\infty$ data were available at high temperatures. Six $x_i^{aq}$ values at temperatures of 313 K and below were combined with the $k_H$ and $\gamma_i^\infty$ data in order to extend the temperature ranges of the $k_H$ and $\gamma_i^\infty$ regressions. At these low temperatures for this compound, $x_i^{aq}$ and SOLC are small so the assumptions required to use Equations 4.1 and 4.4 are valid. When SOLC data were not available for some compounds, family trends were used to estimate the validity of the assumptions required to use Equations 4.1 and 4.4 in order to determine the classifications of the regressions. If data were available that fell within reasonable limits of the assumptions used for the thermodynamic relationships, then the temperature dependent regressions were labeled as “Smoothed”. If there was any doubt concerning the validity of the assumptions, the regressions were labeled as “Predicted” or “Exp&Pred” (Experimental and Predicted) depending on the amount of data available for the different properties.

Recommended constant values were determined for the three properties from the temperature-dependent regressions evaluated at 298.15 K. These values were entered as new constant values and classified as “Smoothed” or “Predicted” depending on if the temperature-dependent regression was classified as “Smoothed” or “Predicted”, respectively.

At the end of the Mathcad® sheets, there were multiple output files linked to Microsoft Excel®. Information determined from the data analysis process (i.e. acceptance, temperature-dependent coefficients, recommended constant values, assigned errors for literature datasets, etc.) were exported to Microsoft Excel®. The Microsoft Excel® file was then used to directly update the Microsoft Access® database. This procedure was different than the update procedure used in DIPPR® 801. With the DIPPR® 801 procedure, values are overwritten in the database with the updated information. However, with the 801E database, the information was updated and not overwritten in order to save the original values and units.

All of the converted data used to obtain the regressions were added to the database and labeled as “Derived”. The notes contain the references from which they were derived. This allows a user to view all of the values that were used to obtain the regression including values that were calculated from other properties.

### 4.3.1 Error Calculations

Linear regression statistics and propagation of error were used to determine the uncertainty of the temperature-dependent regressions. Table 4.5 summarizes the error analyses used in this study. The $\gamma_i^\infty$ regressions and resulting errors were derived from the $k_H$ regressions. The confidence intervals were initially determined on a natural log scale, but they were converted to a normal scale in order to determine uncertainty assignments. In some instances, the uncertainty assignments were adjusted based on additional factors. Examples of this are given later in this section. All of the regressions assumed constant variance. In reality, some data are more reliable than others. Efforts were made to only include the best data in each regression so that the assumption of constant variance was valid.

Table 4.5: Summary of uncertainty determinations for temperature-dependent regressions

| Property | Regression | Error Analysis | Assumptions |
|---|---|---|---|
| $k_H$ | Least squares | 95% confidence intervals of the mean (determined by regression) | Constant variance |
| $\gamma_i^\infty$ | Thermodynamically derived from $k_H$, $P_i^{sat}$, and $\Psi$ | Propagation of error | Constant variance |
| $x_i^{aq}$ | Least squares | 95% confidence intervals of the mean (determined by regression) | Constant variance |

Confidence intervals determined in this manner are not constant over the entire temperature range. Confidence intervals are larger at the minimum and maximum temperatures. In addition, for compounds that cover solid and liquid regions, the uncertainty in $\gamma_i^\infty$ tends to be larger over the solid region versus the liquid region due to uncertainty in $\Psi$. In the DIPPR® 801 database, confidence intervals are assigned to the entire regression. To be consistent with the 801 database format, single uncertainties were assigned. This was accomplished by a weighted average. First, the average absolute upper and lower percent uncertainties, *s*, were calculated at every temperature for each experimental data point, *j*,

$$s_j = \frac{\left|\%Error_{up}(T_j)\right| + \left|\%Error_{down}(T_j)\right|}{2}, \qquad 4.18$$

where *%Error* is the percent difference between the 95% confidence interval of the mean and the regression value. If there were *N* points at a single temperature, then the uncertainty was calculated *N* times. These resulting uncertainties were then averaged,

$$s = \frac{\sum_j s_j}{N_{total}}, \qquad 4.19$$

where $N_{total}$ is the total number of experimental points used to obtain the regression. This resulted in greater weight for the temperatures where there were more experimental values. These weighted absolute uncertainties were then converted to DIPPR® 801 uncertainty ranges. The DIPPR® uncertainty options are < 0.2%, < 1%, < 3%, < 5%, <10%, < 25%, < 50%, < 100%, and > 100%. As an example, if $s$ = 2.7%, the uncertainty for the regression was labeled as < 3%.

When data were only available for one property, uncertainties were initially calculated as outlined in Table 4.5. The uncertainties of the derived property regressions were then compared to the error assigned to the regression of the original data. The derived property uncertainty was kept if it was greater than or equal to the error of the original property data. If it was smaller, it was changed to match the uncertainty of the original property. For example, if $k_H$ and $\gamma_i^{\infty}$ regressions were determined from $x_i^{aq}$ data and the uncertainty assigned to the $x_i^{aq}$ regression was < 25%, the smallest uncertainty assigned to the $k_H$ and $\gamma_i^{\infty}$ regressions was < 25%.

When data were only available from one reference, an uncertainty was calculated from the regression, and this was compared to the reported author uncertainty. The largest uncertainty of the two was reported in the database. For example, with ethyl mercaptan the uncertainty obtained from the $k_H$ regression was < 5%. However, the uncertainty reported by the author for the dataset was < 10%, so the uncertainty of the regression was changed to < 10%.

Uncertainties were assigned to the individual datasets based on the regression uncertainty. Figure 4.4 shows an example of the error calculation for an experimental data point. Each data point is at the same temperature. The points are spread along the x-axis for viewing purposes. The correlation value and uncertainty are shown along with an experimental value (shown twice). The uncertainty of the experimental value can be calculated in two different ways as shown in the figure. The uncertainty can be taken as the difference between the experimental and correlated values or the difference between the experimental value and uncertainty limit of the correlated value. The latter calculation was used in this study. The absolute uncertainties of all of the data points within a dataset were averaged to assign an overall uncertainty to the dataset. The lowest possible uncertainty for a dataset was defined as being the uncertainty assigned to the regression. For example, if a regression was assigned an uncertainty of < 10% and the difference between the experimental data and regression values is 3%, the uncertainty of the dataset was labeled as < 10%.

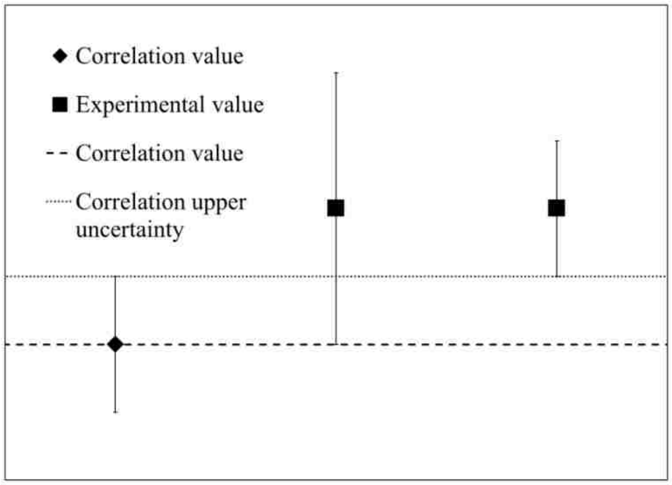

Figure 4.4: Uncertainty determination of experimental datasets

### 4.3.2 Critical Solution Temperatures

This section discusses compounds with upper or lower critical solution temperatures. Table 4.6 gives the total number of compounds per chemical family with critical solution behavior that were evaluated in this study. For the compounds with critical solution behavior, the actual critical temperatures were not determined. The determination of the actual critical point would involve the evaluation of $x_i^{aq}$ and SOLC data which was beyond the scope of this study. Term "E" in DIPPR® Equations 5000 and 6000 (see Table 4.3) was assigned a value (an approximate critical temperature) based on the available $x_i^{aq}$ data. This allowed the remaining coefficients to be found using linear regression. Values should be extrapolated from temperature-dependent equations with caution for all properties discussed in this paper. Errors can result from extrapolation, especially for $x_i^{aq}$. Some of the more interesting behaviors encountered in this study are discussed below.

Table 4.6: Chemical families with evaluated compounds exhibiting critical solution behavior

| Chemical Family: Number Evaluated Compounds/Type of Critical Solution Behavior[a] | |
|---|---|
| Aldehydes: 1/UCST | Nitriles: 2/UCST |
| Aromatic Alcohols: 12/UCST | Nitroamines: 1/UCST |
| Aromatic Amines: 2/LCST | Other Aliphatic Alcohols: 1/UCST |
| Aromatic Carboxylic Acids: 1/UCST | Other Aliphatic Amines: 5/LCST |
| Cycloaliphatic Alcohols: 1/UCST | Other Amines, Imines: 3/LCST |
| Epoxides: 1/UCST | Other Ethers/Diethers: 1/LCST |
| Ketones: 1/UCST | Other Polyfunctional C, H, O: 1/UCST |
| n-Alcohols: 1/UCST | Polyfunctional C, H, O, Halide: 3/UCST |

[a] UCST = Upper Critical Solution Temperature; LCST = Lower Critical Solution Temperature

Figure 4.5 shows $\ln(x_i^{aq})$ data plotted versus inverse temperature for 2-butanol along with the regression obtained in this study. Below 273.15 K (0.00366 $K^{-1}$), the $\ln(x_i^{aq})$ data plateau. The data below 273.15 K were not included in the regression due to the inability of any of the equations in Table 4.4 to model the behavior with these data included. Extrapolation of the regression below 273.15 K would obviously give erroneous $x_i^{aq}$ values.

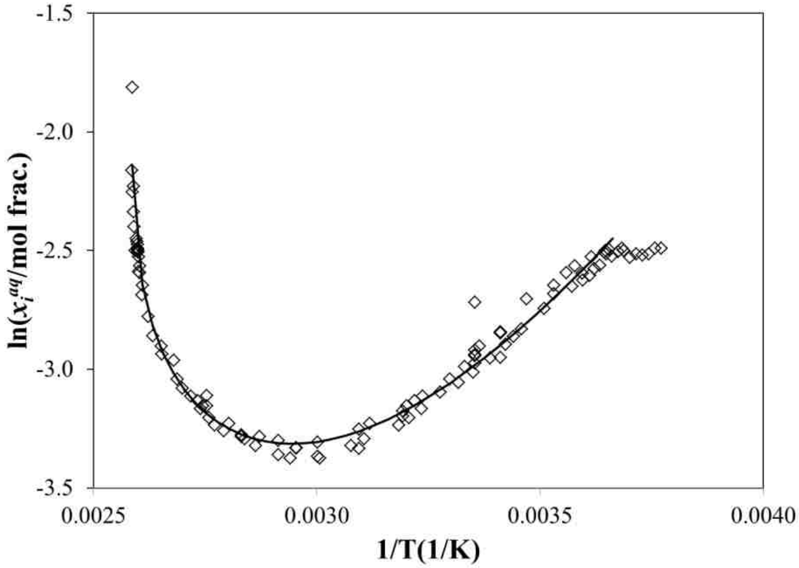

Figure 4.5: 2-Butanol $\ln(x_i^{aq})$ data and regression. References: [55-62]

Figure 4.6 shows $\ln(x_i^{aq})$ data of p-chlorophenol plotted as a function of inverse temperature along with the regression obtained by using DIPPR® Equation 6000. The regression was purposefully extrapolated beyond the maximum temperature in the figure to show the dangers of extrapolation. DIPPR® Equation 6000 is not quite adequate for the $x_i^{aq}$ behavior of *p*-chlorophenol as can be seen by the residual plot in Figure 4.7. The behavior of the residuals suggests that additional or different terms are required to correctly model the temperature-dependence since there is a pattern in the residuals. However, since compounds like this were the exception, DIPPR® Equation 6000 was used anyway. As already mentioned, it was desired to have a generic equation that could apply to multiple compounds. Equations were not developed for individual compounds. The error of the regression for *p*-chlorophenol was taken into account with the regression statistics, and this error is reflected in the assigned uncertainty.

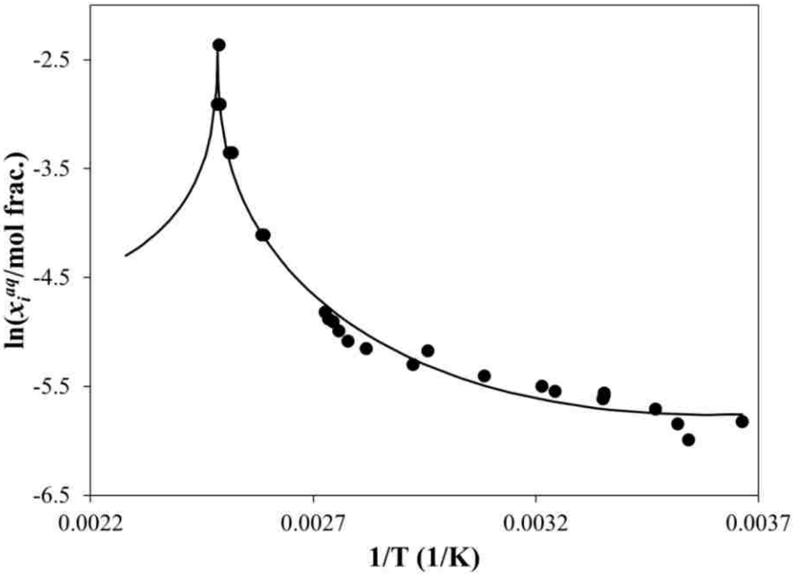

Figure 4.6: $\ln(x_i^{aq})$ data and regression for p-chlorophenol. References: [63-67]

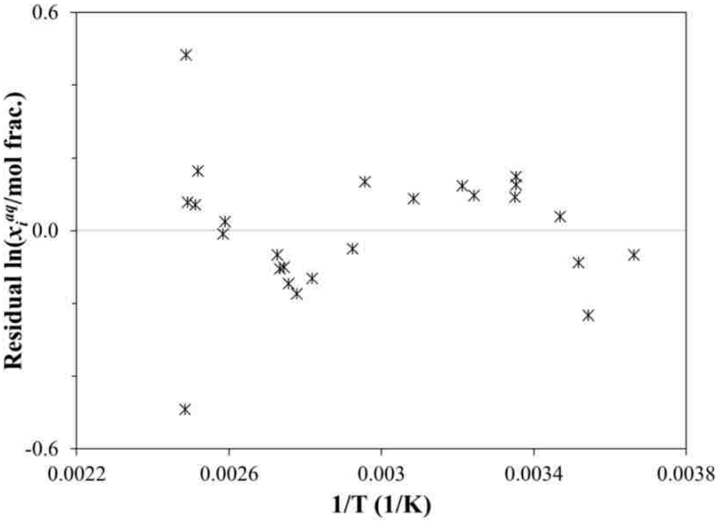

Figure 4.7: Residual plot from p-chlorophenol $\ln(x_i^{aq})$ regression

### 4.3.3 Chemical Family Plots

Chemical family plots of temperature-dependent regressions obtained from experimental data were used to select the best experimental datasets for a compound within the chemical family and qualitatively check the reasonableness of the temperature trends. Temperature-dependent chemical family plots were used throughout this project when enough data were available for similar compounds. Most regressions within a chemical family have varying applicable temperature ranges due to the data available for the individual compounds. Extrapolated values based on experimental data do not always follow the trends of other compounds within the family. When enough chemical family data were available, temperature regressions were modified to change extrapolated behavior to better match the chemical family trends. However, the main concern was ensuring that trends were reasonable over the recommended temperature ranges of the regressions.

Figure 4.8 is a plot of the *n*-alcohol $\ln(x_i^{aq})$ regressions (determined in this study from experimental data) versus inverse temperature starting with 1-butanol. Smaller alcohols were not included because of their miscibility with water. As the number of carbons (#C) increases, $x_i^{aq}$ decreases which is what is expected. 1-Butanol exhibited an upper critical solution temperature in the temperature range of available data. Two regressions are shown for 1-octanol. The C8 regression is based solely on experimental data. As can be seen in the figure, the C8 regression does not follow the same trend as the other *n*-alcohols. A second regression was developed (C8-Exp&Pred) using the experimental data and predicted points based on the family trend. This second regression was accepted.

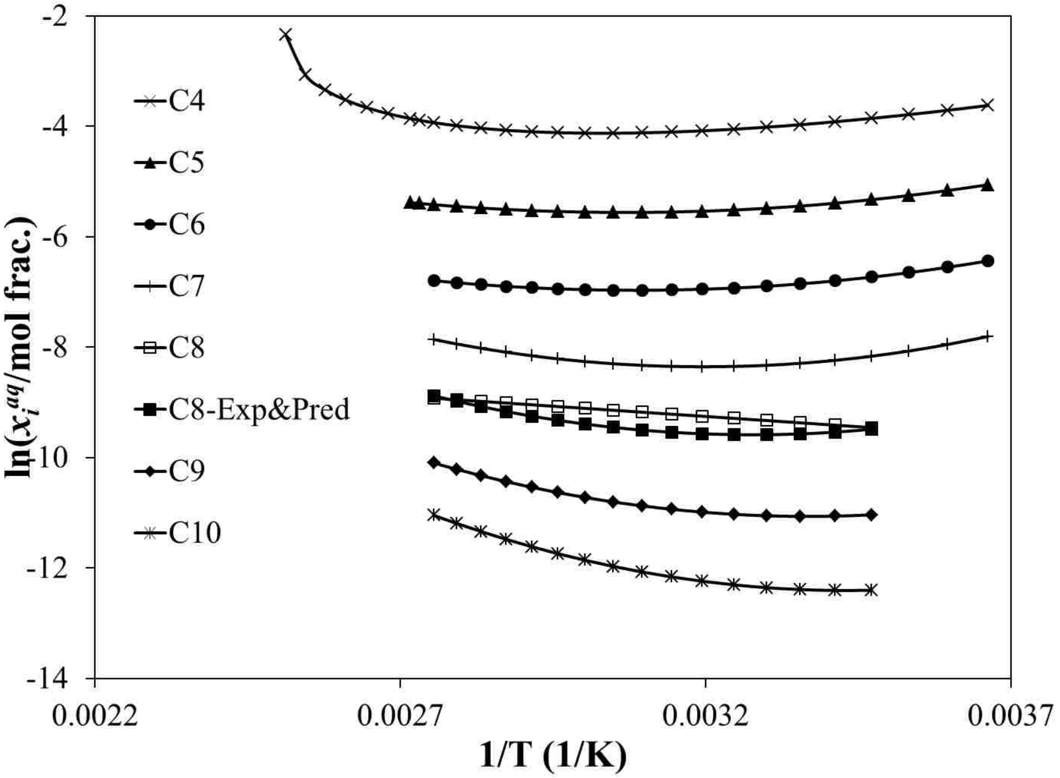

Figure 4.8: *n*-Alcohol ln($x_i^{aq}$) regressions based on experimental data versus inverse temperature. Initial C8 regression based on experimental data (C8) and updated C8 regression based on experimental data and predicted values from the family plot (C8-Exp&Pred) are both shown.

A chemical family plot was used to determine the best $k_H$ and $\gamma_i^\infty$ data for 1-heptanol (C7). Due to C7 SOLC values ranging between 0.285-0.334 mole fraction over the temperature range of 278.15-333.15 K [58, 59], $x_i^{aq}$ data were not included in the $k_H$ and $\gamma_i^\infty$ regressions. However, $x_i^{aq}$ data were still helpful in identifying the best datasets. C7 literature values plotted as ln($k_H$) versus inverse temperature are shown in Figure 4.9. The 1-hexanol and 1-octanol (C6 and C8) $k_H$ regressions were also used to identify the best datasets. The data from reference a [47] and the values reported from one of the experimental methods used in reference c [68] agree with the average of the C6 and C8 regressions (Avg C6 & C8). These two references also agree with the literature $x_i^{aq}$ data. Predicted values from the average of the C6 and C8 regressions at temperatures higher and lower than the available C7 data were included in the regression so the extrapolated behavior better matched the family behavior.

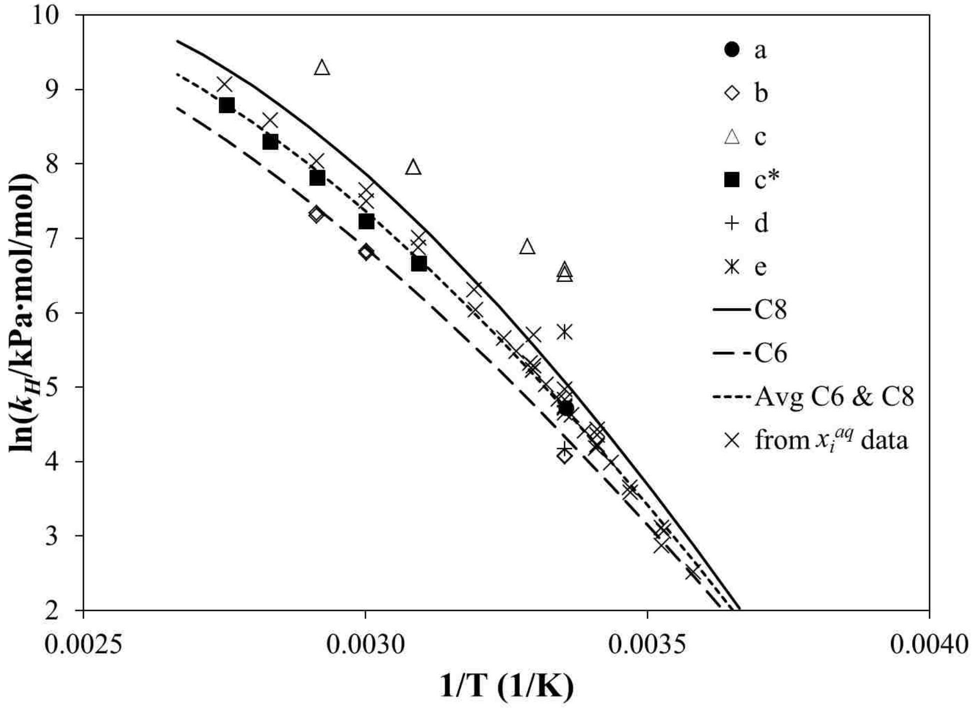

Figure 4.9: 1-Heptanol values plotted as ln($k_H$) versus inverse temperature. 1-Octanol (C8) and 1-hexanol (C6) regressions obtained from experimental data shown along with the average of these two regressions (Avg C6 & C8). References: a [47], b [69], c [68] (*reference reports values using two different experimental methods), d [70], e [71], $x_i^{aq}$ data [44, 72-80]

Figure 4.10 is a plot of ln($\gamma_i^{\infty}$) regressions versus inverse temperature for the *n*-alcohols. Values in the figure are plotted within the recommended temperature ranges of each regression; however, extrapolated trends were considered. Initially all of the regressions were developed based solely on experimental data. The larger *n*-alcohols have fewer data with more scatter than the smaller *n*-alcohols. As a result, the regressions have larger uncertainties. For 1-octanol (C8), curvature was not significant over the temperature range of the data, so extrapolated values did not match the shape of the other compounds. Predicted values were combined with the C8 experimental data to obtain curves for $\gamma_i^\infty$ and $k_H$ (C8-Exp&Pred). As was mentioned, predicted values were also combined with the C7 experimental data to help with extrapolation. The change in the regression due to the predicted points was not as drastic for C7 as with C8, so it is not shown in the plot. As #C increases, $\gamma_i^\infty$ values increase meaning that deviations from ideality are increasing. As the carbon chain grows, the molecules become more hydrophobic.

Figure 4.11 is a plot of the ln($k_H$) regressions for the *n*-alcohols shown over extrapolated temperature ranges. The same data used to obtain the regressions shown in Figure 4.10 were used to obtain the $k_H$ regressions. As was seen with $\gamma_i^\infty$ for 1-octanol, the initial regression based only on experimental data (C8) extrapolated differently from the other compounds. The "8-Exp&Pred regression follows the chemical family trend at higher temperatures. The difference between the $k_H$ temperature-dependent behavior of the C8 and C8-Exp&Pred regressions is very noticeable in Figure 4.11. As with the $\gamma_i^\infty$ values, as #C increases, $k_H$ values increase. However, the influence of temperature is greater on $k_H$ than $\gamma_i^\infty$. It has been noted that changes in $k_H$ are small in a chemical family when compared to $x_i^{aq}$ and $P_i^{sat}$ [19]. This is especially obvious at lower temperatures with the *n*-alcohols. Since $x_i^{aq}$ and $\gamma_i^\infty$ are inversely related for liquids (see Equation 4.4), then changes in $\gamma_i^\infty$ will also be larger in a chemical family than changes in $k_H$. These trends are also observed with the *n*-alcohol regressions.

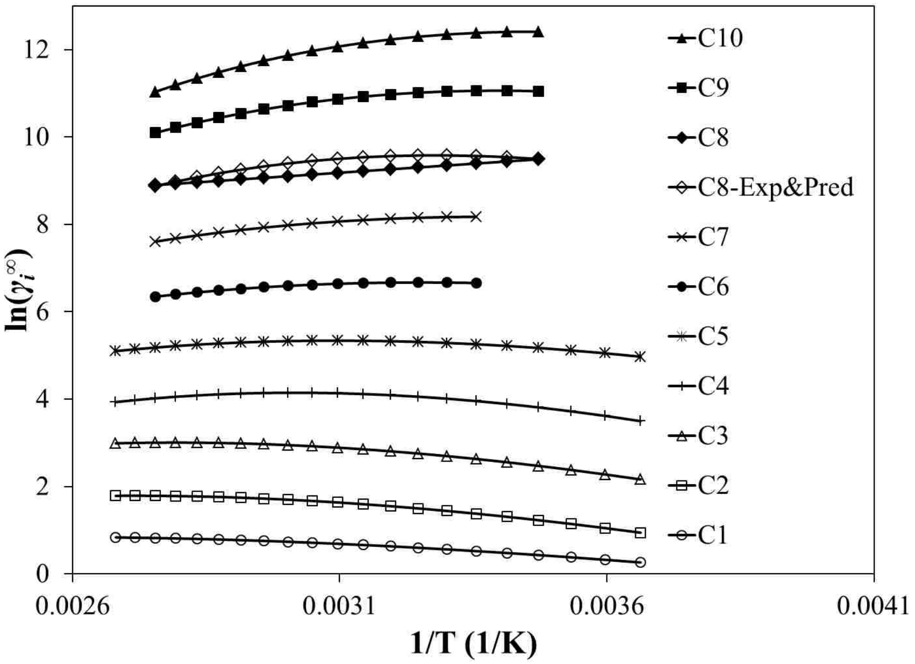

Figure 4.10: *n*-Alcohol $\ln(\gamma_i^\infty)$ regressions based on experimental data versus inverse temperature

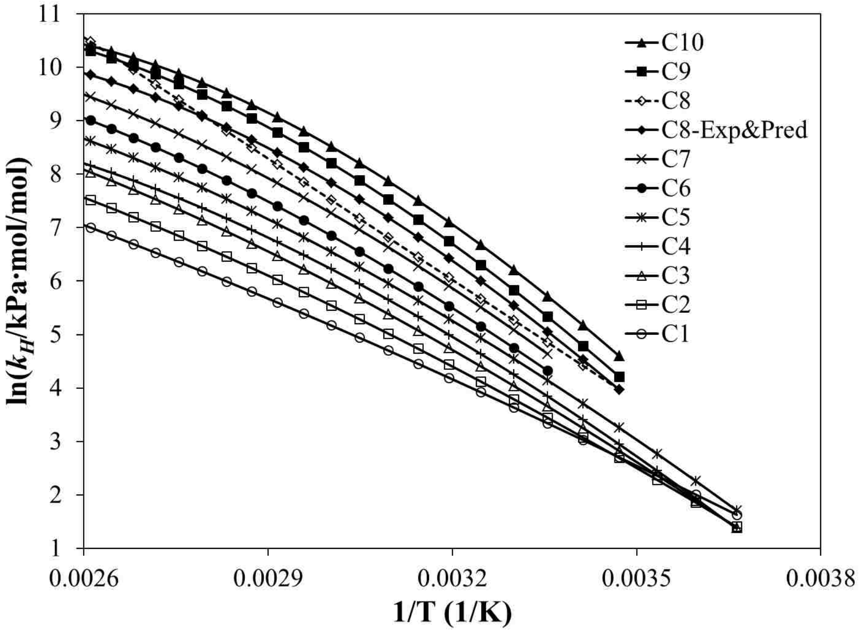

Figure 4.11: *n*-Alcohol $\ln(k_H)$ regressions based on experimental data versus inverse temperature

### 4.3.4 Other Data Analysis Notes

For some compounds, $\gamma_i^\infty$ or $k_H$ values are reported from $x_i^{aq}$ measurements, but the $P_i^{sat}$ and/or $\Psi$ values used in the literature were significantly different from those calculated in this study. In these instances, $\gamma_i^\infty$ and $k_H$ values were recalculated from the original $x_i^{aq}$ values using DIPPR®801 properties and the values reported in the literature were not used.

## 4.4 Constant Values

Temperature-dependent data are not available for every compound, so chemical family plots were used to evaluate compounds with data only available at 298.15 K. Plots of the natural log of $x_i^{aq}$ or $\gamma_i^\infty$ often are a linear function of carbon number (#C) [81, 82]. These plots use a group contribution approach (discussed in more detail in Section 7.1). If a plot is created in which a unit on the x-axis represents the addition of a molecular group (which in this study was typically chosen to be $-CH_2-$), the property will change in incremental values with the number of groups. If there is a functional group that is similar to all compounds, it does not have to be explicitly included on the x-axis. For example, a linear trend can be observed for *n*-alcohols where the x-axis only takes into account the #C. Since all compounds have a hydroxyl group on C1, this functional group is inherently accounted for in the plot. These types of family plots were used to either smooth values as a function of #C or designate the best experimental values based on the family trend. The property that was chosen for the family plots was the property that had the best linear correlation (highest $R^2$ value) for the natural log of the property plotted as a function of #C.

### 4.4.1 Chemical Family Plot Regressions

Within a chemical family, some of the compounds had enough data to perform temperature-dependent evaluations (see Section 4.3) while other compounds only had data at a single temperature. In these instances, “Smoothed” values (determined by evaluating the temperature-dependent regressions at 298.15 K) were combined with the available literature data at 298.15 K of the unevaluated compounds to obtain a regression of the natural log of a property as a function of #C. Recommended values were then determined for each unevaluated #C using the regression. This method was used when most of the compounds in a chemical family already had recommended values from evaluating temperature-dependent data. In other instances, all of the original data at 298.15 K were used within a chemical family to obtain a regression of the natural log of a property as a function of #C. Since every chemical family was handled uniquely due to the availability of data, notes about the data used to determine recommended values from family plots were included in the database with the “Smoothed” values. Examples of this data evaluation process and chemical families with interesting behavior are included below.

The constant value family plot for the 1-alkenes is an example of using all of the literature data in the evaluation process. Temperature-dependent evaluations were not performed for any of the liquid 1-alkenes due to the limited amount of temperature-dependent data. Literature $k_H$ and $x_i^{aq}$ data at 298.15 K for the 1-alkenes are plotted as $\ln(x_i^{aq})$ versus #C in Figure 4.12. The data show a linear relationship between $\ln(x_i^{aq})$ and #C ($R^2 = 0.997$). A linear regression was used to obtain recommended $x_i^{aq}$ values at 298.15 K and labeled as “Smoothed” for each #C of the chemical family. The 95% confidence intervals of the mean (as determined by the regression) were used to determine the uncertainty of the “Smoothed” values. Values were predicted for C10-C14 by interpolation and labeled as “Predicted”. The recommended 1-

alkene $x_i^{aq}$ values were used to determine values for $k_H$ and $\gamma_i^{\infty}$ using the relationships in Section 4.1. Figure 4.13 is a plot of the ln($k_H$) values for this same family obtained from the “Smoothed” and “Predicted” values of this study compared to the predicted values using the HENRYWIN bond-contribution method [83]. There is good agreement between the HENRYWIN values and the values obtained in this study.

“Smoothed” values from the temperature-dependent evaluations of this study were used in combination with literature data to evaluate constant value data for some chemical families. For the 1-iodoalkanes, temperature-dependent data were evaluated for methyl iodide, ethyl iodide, and *n*-propyl iodide. However, *n*-butyl iodide and *n*-hexyl iodide each only have one reported experimental value. The “Smoothed” values obtained from the temperature-dependent regressions were used with the two literature experimental values to determine “Smoothed” values for *n*-butyl and *n*-hexyl iodide. A plot of ln($k_H$) versus #C for the five points shows a linear trend ($R^2 = 0.9866$). However, when the data are plotted as ln($\gamma_i^{\infty}$) versus #C, there is a superior linear trend ($R^2 = 0.9995$). Because of this, a regression was performed using ln($\gamma_i^{\infty}$) versus #C to obtain “Smoothed” $\gamma_i^{\infty}$ values for *n*-butyl iodide and *n*-hexyl iodide. These “Smoothed” values were converted to $k_H$ and $x_i^{aq}$. Figure 4.14 shows the “Smoothed” $k_H$ values obtained from the temperature-dependent regression, the two experimental points of the unevaluated compounds in terms of $k_H$, the “Smoothed” $k_H$ values obtained from the constant value family plot, and the predicted $k_H$ values from the HENRYWIN bond-contribution method [83].

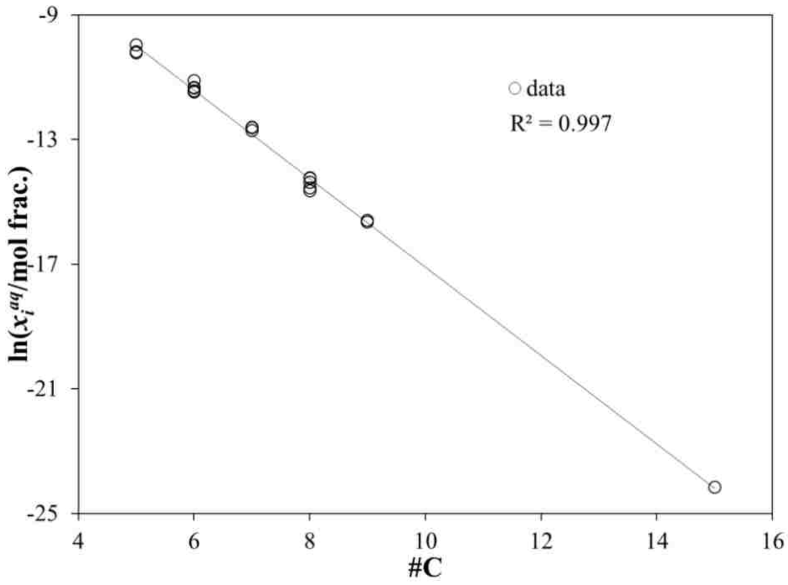

Figure 4.12: 1-Alkene $k_H$ and $x_i^{aq}$ data at 298.15 K plotted as ln($x_i^{aq}$) versus carbon number (#C). References: [47, 72, 84-87]

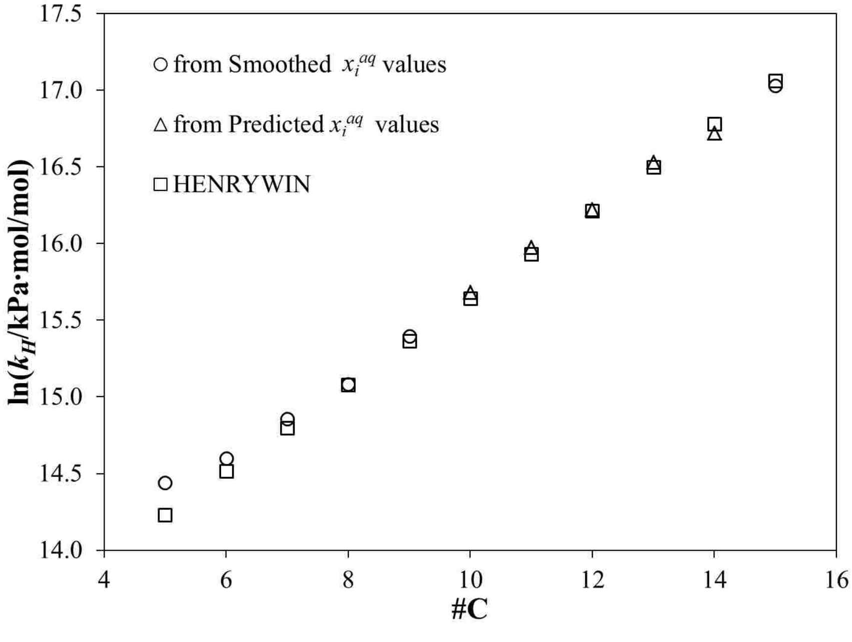

Figure 4.13: 1-Alkene ln($k_H$) values at 298.15 K from this study ("Smoothed" and "Predicted") and HENRYWIN bond-contribution prediction method [83] plotted as a function of carbon number (#C)

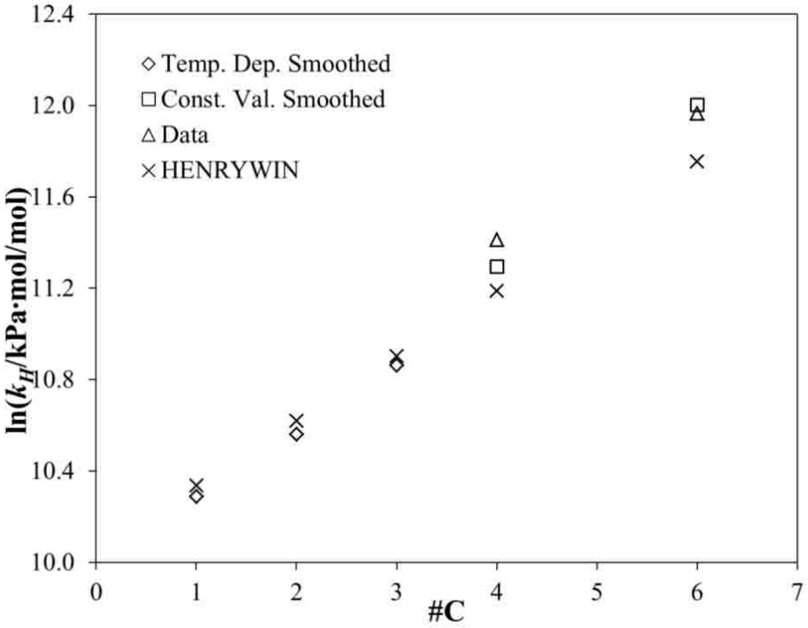

Figure 4.14: 1-Iodoalkane ln($k_H$) values at 298.15 K from temperature-dependent regressions (Temp. Dep. Smoothed), constant value family plot (Const. Val. Smoothed), the literature (data) [47], and HENRYWIN bond-contribution method [83] plotted as a function of carbon number (#C)

Figure 4.15 shows "Smoothed" values obtained from temperature-dependent evaluations for the C4-C10 *n*-alcohols and literature values for the C11 and larger *n*-alcohols. Data at temperatures ranging between 277.15 K and 307.15 K were included due to the limited data available for the larger compounds. The values that are at 298.15 K have solid backgrounds. Possible reasons for the scatter in the literature data include difficulties with accurately measuring small concentrations, the addition of trace amounts of salts by some authors in order to prevent microbial degradation of the alcohol (references c [88] and f [89]), and varying temperatures ($x_i^{aq}$ values are expected to be smaller at lower temperatures). The C16 and C17 data of reference d [90] suggests that the $x_i^{aq}$ values eventually plateau as a function of #C. However, the authors of reference d [90] report that the C17 $x_i^{aq}$ value is less than or equal to the value shown on the plot. The actual $x_i^{aq}$ was below the detection limits of the method used by the authors, so this point cannot be given serious weight. The values from the other authors do not provide any evidence of the $x_i^{aq}$ values plateauing before C18. Because of all of these factors, $x_i^{aq}$ values for C11-C18 were predicted by extrapolating the regression obtained from the "Smoothed" values (shown in the figure).

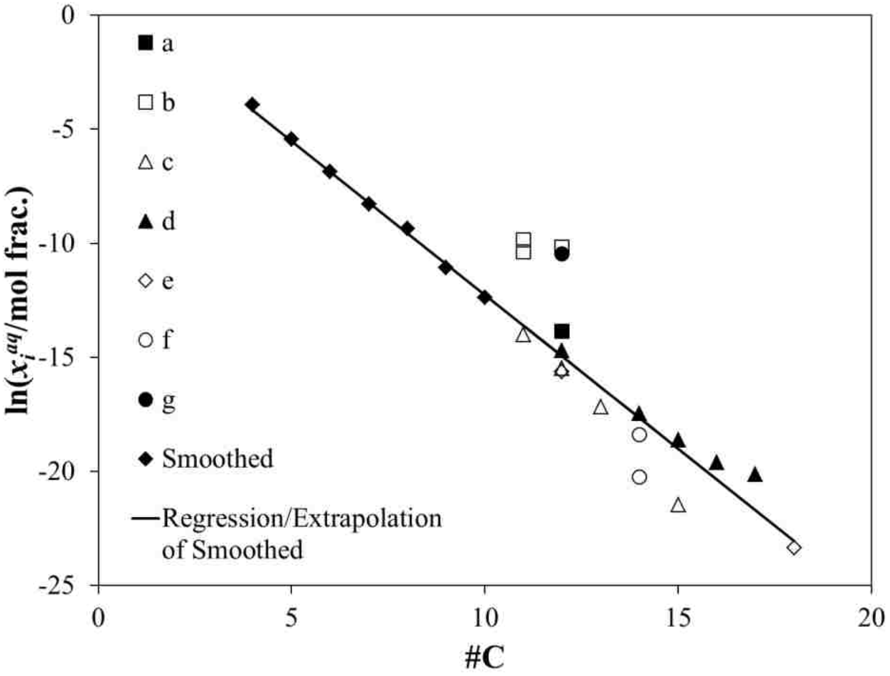

Figure 4.15: *n*-Alcohol "Smoothed" values from temperature-dependent evaluations and literature values plotted as ln($x_i^{aq}$) versus carbon number (#C). Solid symbols represent values at 298.15 K. Other values are at temperatures ranging from 277.15 K to 307.15 K. References: a [70], b [91], c [88], d [90], e [92], f [89], g [93]

Figure 4.16 shows the "Smoothed" values from temperature-dependent evaluations and the literature values above C10 for the *n*-alkanes. There is a large degree of scatter in reported values due to the difficulties in accurately measuring the $x_i^{aq}$ values of the larger *n*-alkanes due to problems caused by adsorption, contamination, and dectection limitations. Tsonopoulos [81] has noted that ln($x_i^{aq}$) for the *n*-alkanes is a linear function of #C up until *n*-nonane. As #C increases beyond C9, ln($x_i^{aq}$) continues to decrease but at a smaller rate. Most of the experimental data indicate that the there is an eventual plateau in $x_i^{aq}$ values. One theory is that the folding of the larger chain *n*-alkanes causes this plateau. Ferguson et al.[94] disagree with this theory and claim that the experimental data are erroneous. They used molecular dynamic simulations to study the $x_i^{aq}$ of *n*-alkanes and found that there is an exponential decrease in $x_i^{aq}$ up to C20. This theory better matches the trend observed with the *n*-alcohols (Figure 4.15). Due to the agreement of the molecular simulations and the *n*-alcohol trend, the data of Tolls et al. [95] (points are highlighted in Figure 4.16) were recommended in this study. Future experimental work would be helpful in better understanding this chemical family trend.

Figure 4.17 shows "Smoothed" and literature $x_i^{aq}$ values for the *n*-alkylbenzenes plotted as a function of #C. Tsonopolous has noted slight curvature as ln($x_i^{aq}$) data are plotted as a function of #C for the *n*-alkylbenzenes [82]. Because of this, a quadratic equation was used to smooth the data instead of linear equation. The value at C19 suggests that the quadratic trend does not continue after C16. The $x_i^{aq}$ values of large hydrocarbons are difficult to measure due to the small concentration, so more $x_i^{aq}$ values of the large *n*-alkylbenzenes need to be measured in order to confidently understand the curvature after C16. "Smoothed" values obtained from temperature-dependent regressions were included in the constant value regression for C6-C12. The available data point at C16 was also included, but the data points at C13 and C14 were rejected because they do not agree with the family plot. Values for C13-C16 were determined from smoothing these combined values.

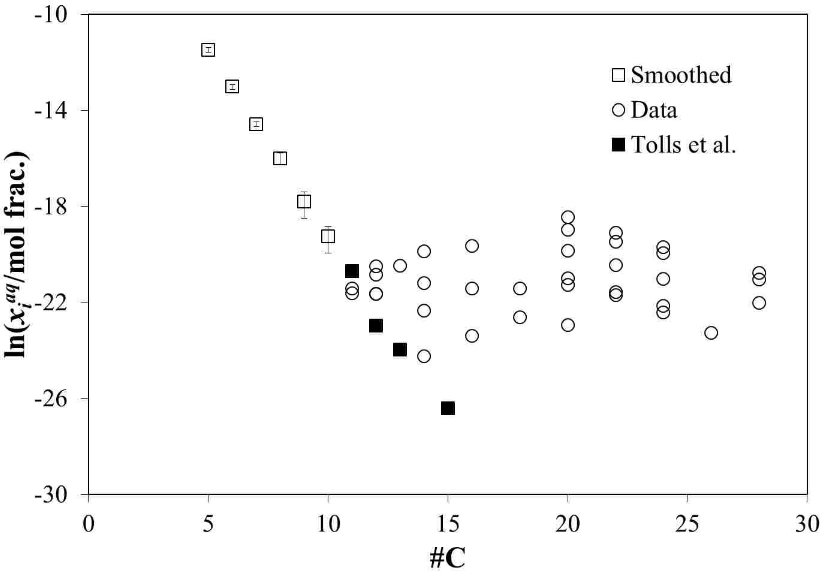

Figure 4.16: *n*-Alkane "Smoothed" values from temperature-dependent evaluations and literature (Data) $x_i^{aq}$ values at 298.15 K. References: [85, 95-104]

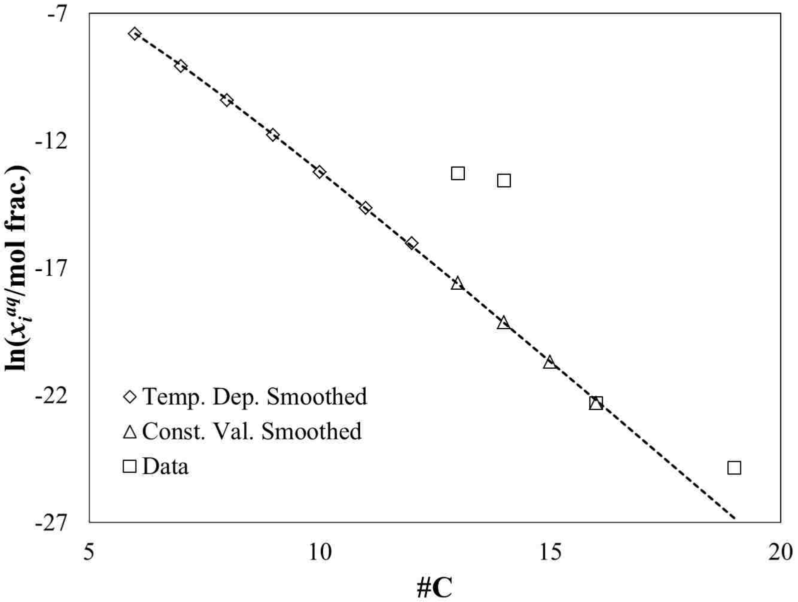

Figure 4.17: *n*-Alkylbenzene $\ln(x_i^{aq})$ values at 298.15 K from temperature-dependent regressions (Temp. Dep. Smoothed), constant value family plot (Const. Val. Smoothed), and the literature (Data) plotted as a function of carbon number (#C). References: [105, 106]

When analyzing the di-*n*-alkyl phthalates, only three of the compounds (dimethyl, diethyl, and di-*n*-butyl phthalates) had temperature-dependent data. These three phthalates were evaluated using the procedure discussed in Section 4.3. The remaining phthalates only have literature $x_i^{aq}$ data at ambient conditions. Figure 4.18 is a plot of $\ln(x_i^{aq})$ at 298.15 K as a function of the number of carbons on the alkyl chains (#C). The linear relationship between $\ln(x_i^{aq})$ and #C was used to provide recommended values for di-*n*-propyl and di-*n*-hexyl phthalates, #C = 6 and #C = 12, respectively. A linear regression was performed with the temperature-dependent "Smoothed" values and the data shown in Figure 4.18. Two literature values were rejected because they did not follow the linear relationship like the remaining data. This regression was used to determine "Smoothed" values for di-*n*-propyl and di-*n*-hexyl phthalates.

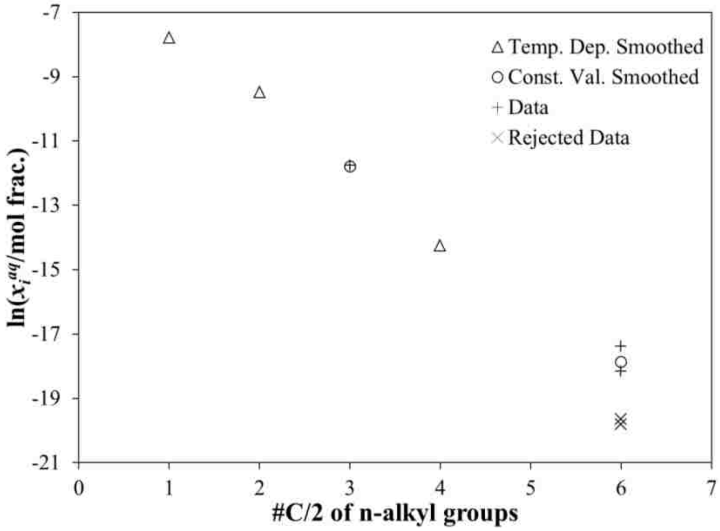

Figure 4.18: di-*n*-Alkyl phthalate $\ln(x_i^{aq})$ values at 298.15 K from temperature-dependent regressions (Temp. Dep. Smoothed), constant value family plot (Const. Val. Smoothed), and the literature (Data and Rejected Data) plotted as a function of the number of carbons on the alkyl chains (#C). References: [107-115]

As in other instances, Equations 4.1 and 4.4 were used with the "Smoothed" $x_i^{aq}$ values to calculate $k_H$ and $\gamma_i^\infty$, respectively. A plot of $\ln(k_H)$ versus #C for the di-*n*-alkyl phthalates yields a surprising trend, shown in Figure 4.19. The values from this study do not show a linear trend like the bond-contribution values predicted by HENRYWIN [83]. Data for diethyl phthalate (#C = 4) were reviewed in an effort to identify potential explanations.

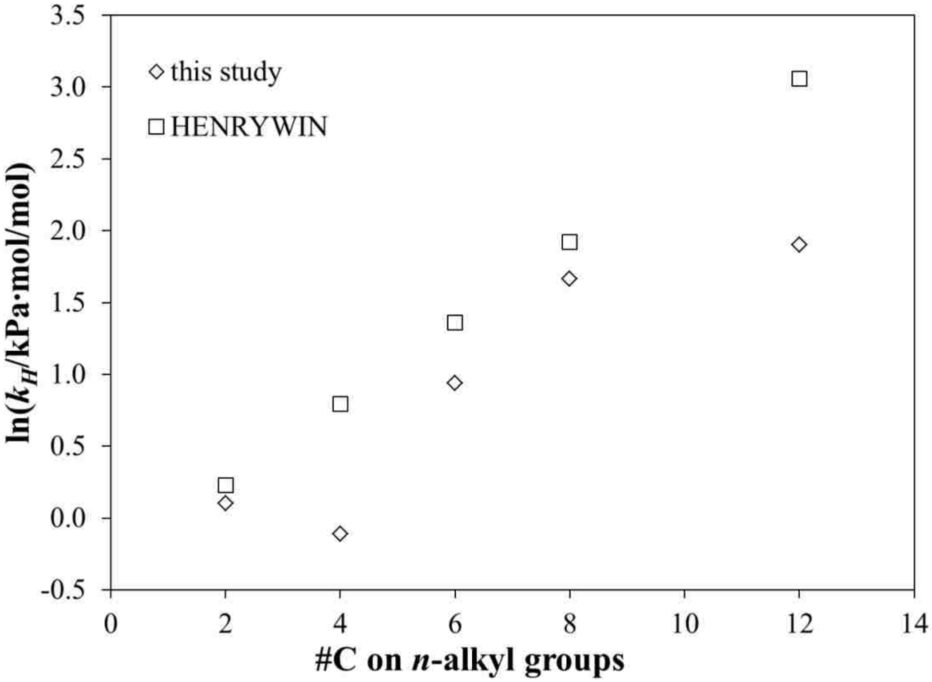

Figure 4.19: di-*n*-Alkyl phthalate "Smoothed" $\ln(k_H)$ values at 298.15 K from this study and from HENRYWIN[83] bond-contribution method

The literature data for diethyl phthalate plotted as $\ln(k_H)$ are shown in Figure 4.20. The experimental value reported in HENRYWIN was calculated from the $x_i^{aq}$ value reported by Howard et al. [110] (reference (e) in the figure). However, the $P_i^{sat}$ value used by HENRYWIN ($2.8 \cdot 10^{-4}$ kPa) to calculate $k_H$ is different from the DIPPR® 801 $P_i^{sat}$ value ($6.64 \cdot 10^{-5}$ kPa). The experimental value reported in HENRYWIN is shown on Figure 4.20 with the bond-contribution value. Both HENRYWIN values are significantly different from the values used in this study. Values in this study are considered superior due to the reviewed $P_i^{sat}$ values available in DIPPR® 801. As can be seen by this example, the quality of $k_H$ values determined using $x_i^{aq}$ is largely dependent on the quality of $P_i^{sat}$ values used.

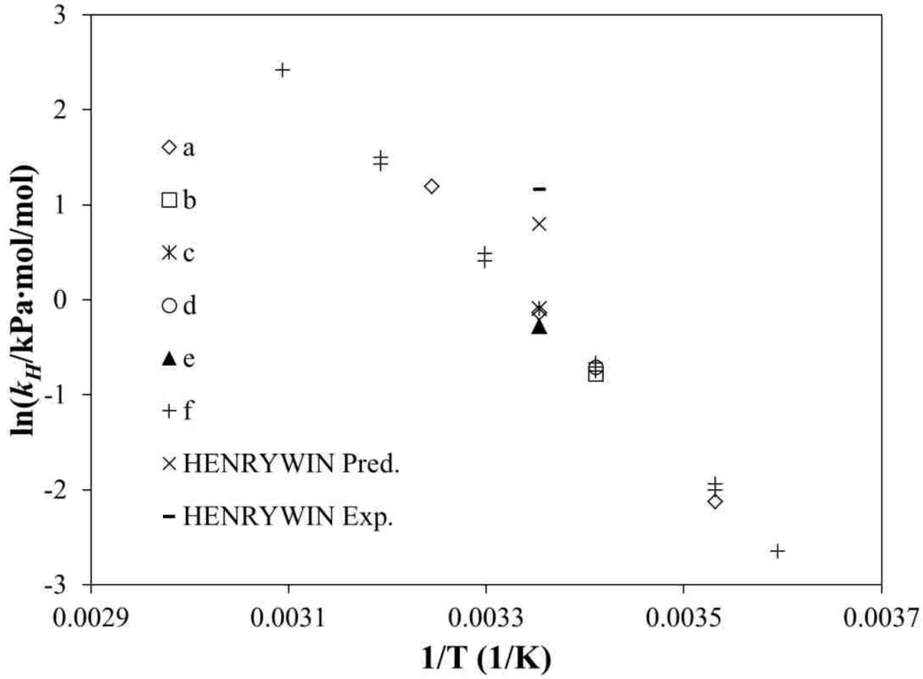

Figure 4.20: Literature data of diethyl phthalate at 298.15 K plotted as $\ln(k_H)$ compared with HENRYWIN bond-contribution value and reported experimental value [83]. References: a [111], b [116], c [109], d [112], e [110], f [107]

The discrepancy between $P_i^{sat}$ values for diethyl phthalate does not fully explain the interesting $k_H$ trend observed in this study. Taking the natural log of Equation 4.1 results in

$$\ln(k_H) = \ln(P_i^{sat}) - \ln(x_i^{aq}) . \qquad 4.20$$

Equation 4.20 explains how a nonlinear trend is obtained from two relatively linear trends. Figure 4.21 shows ln($P_i^{sat}$) and ln($x_i^{aq}$) on the same plot. Both properties have linear trends with $R^2 > 0.99$. For the two smallest compounds, ln($P_i^{sat}$) and ln($x_i^{aq}$) are very similar to each other meaning that ln($k_H$) is close to 0. For all of the compounds except diethyl phthalate, ln($P_i^{sat}$) is larger than ln($x_i^{aq}$) resulting in a positive ln($k_H$). For diethyl phthalate, ln($P_i^{sat}$) is slightly smaller than ln($x_i^{aq}$) which leads to a negative ln($k_H$). If ln($P_i^{sat}$) and ln($x_i^{aq}$) were completely linear functions of #C, then ln($k_H$) would exhibit a completely linear trend. The values obtained in this study were accepted despite the unusual trend. Either more experimental data are necessary to find a better trend, or $k_H$ values for this chemical family are not modeled very well using a group contribution approach.

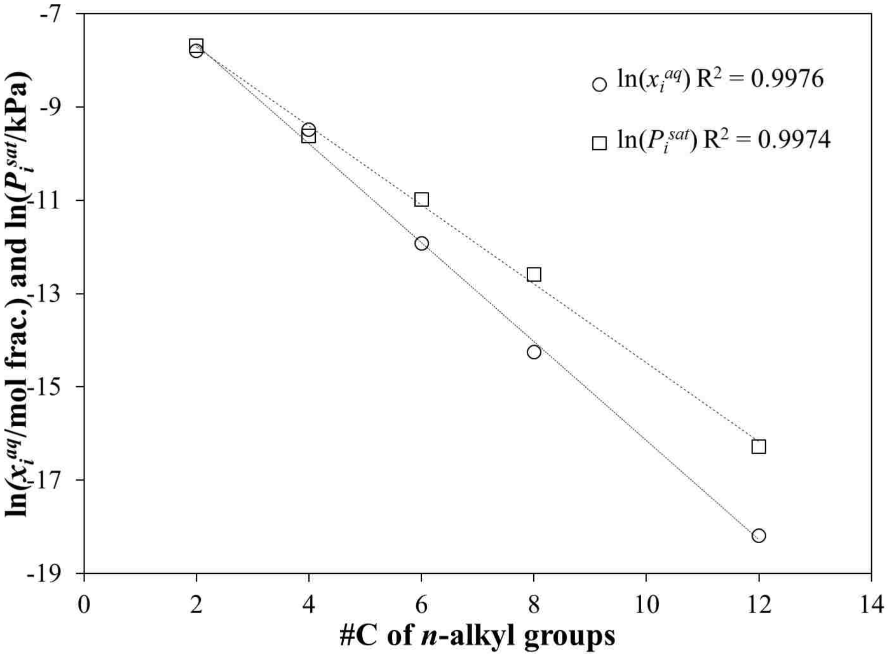

Figure 4.21: Smoothed ln($x_i^{aq}$) and ln($P_i^{sat}$) [117] of di-*n*-alkyl phthalates at 298.15 K

Temperature-dependent $k_H$ and $x_i^{aq}$ data were available for the C5, C6, and C8 cycloalkanes, allowing for the determination of temperature-dependent regressions. Only limited $x_i^{aq}$ data are available for C7. Values obtained from the regressions at 298.15 K were analyzed with the data for C7. A $\ln(x_i^{aq})$ family plot was used to predict $x_i^{aq}$ for C7 which was then used to calculate $k_H$ and $\gamma_i^{\infty}$ values for this compound. (The reported $x_i^{aq}$ value at 298.15 K did not agree with the family plot, so it was rejected.) Similarly, for the C5-C8 cycloalkenes, all but C7 had temperature-dependent $k_H$ and $x_i^{aq}$ values. A family plot showed that the reported $x_i^{aq}$ value for C7 at 298.15 K agrees with the values for the other compounds. This $x_i^{aq}$ value was accepted and used to determine $k_H$ and $\gamma_i^{\infty}$at 298.15 K. The $\ln(x_i^{aq})$ values for the cycloalkanes and cycloalkenes are shown in Figure 4.22 with $\ln(P_i^{sat})$ values shown on the same figure. The cycloalkanes and cycloalkenes both become less soluble in water as #C increases. The cycloalkanes are less soluble than the cycloalkenes which is because of the presence of the double bond in the cycloalkenes.

Figure 4.23 shows cycloalkane and cycloalkene $\ln(k_H)$ values accepted from this study compared to HENRYWIN bond-contribution values [83]. The values in this study do not increase with #C as predicted by HENRWIN; the values are fairly constant for each of the families. This is explained by the $\ln(x_i^{aq})$ and $\ln(P_i^{sat})$ trends shown in Figure 4.22. The two properties have fairly parallel trends to each other for each chemical family (and even between families). The difference between two parallel lines is a constant. Since, $\ln(k_H)$ is the difference between these parallel trends (see Equation 4.20), the $\ln(k_H)$ values are fairly constant. As shown with the *n*-alcohol example (Section 4.3.3), the difference between $k_H$ values within a chemical family is much smaller than the difference in $x_i^{aq}$ or $\gamma_i^{\infty}$.

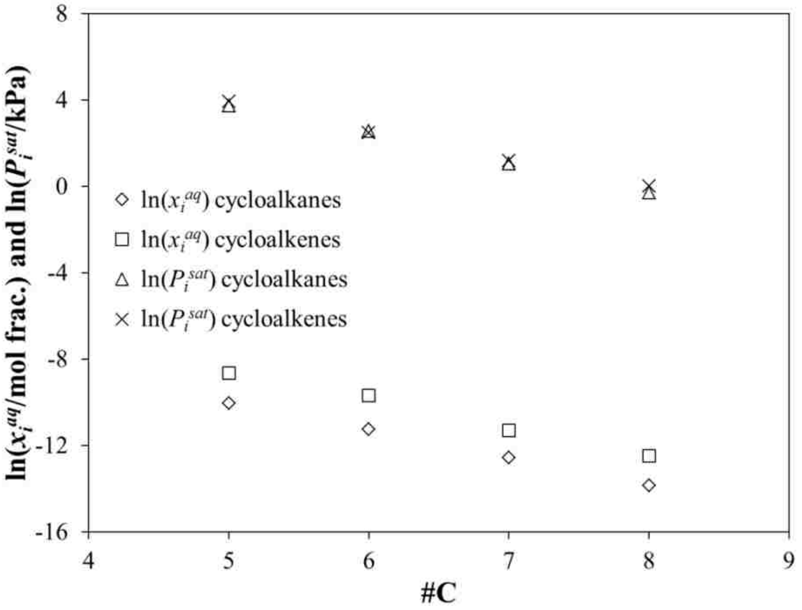

Figure 4.22: Cycloalkane and cycloalkene ln($x_i^{aq}$) and ln($P_i^{sat}$) values at 298.15 K plotted as a function of carbon number (#C). References: [86, 117]

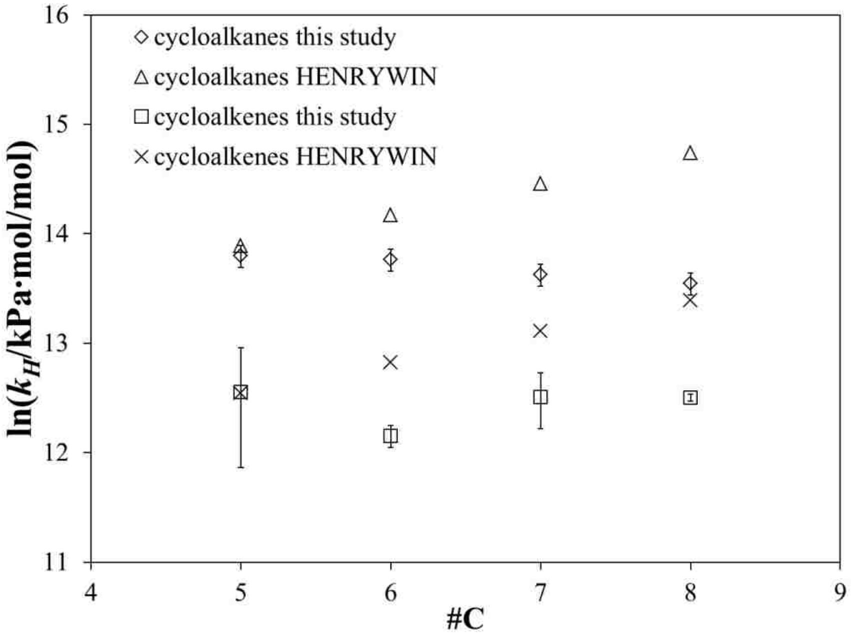

Figure 4.23: Cycloalkane and cycloalkene ln($k_H$) values at 298.15 K compared to HENRYWIN bond-contribution values [83]

### 4.4.2 Averaging

For some compounds it was difficult or impossible to do a family plot due to the unavailability of data for compounds with similar structures. For some compounds, the reported values at 298.15 K were averaged when multiple reported values are in good agreement with each other. In this case, the error was related to the standard deviation of the average. For example, $k_H$ and $\gamma_i^\infty$ values are only available for triethylamine at 298.15 K. These values look reasonable compared to $x_i^{aq}$ data at that temperature (Figure 4.24). However, $x_i^{aq}$ data were not used to obtain temperature-dependent equations for $k_H$ and $\gamma_i^\infty$ due to the relatively high SOLC and the lower critical solution behavior. Instead, averages were taken of the available $k_H$ and $\gamma_i^\infty$ values after conversion to the same property. The standard deviation of the literature data at this temperature is less than 5%.

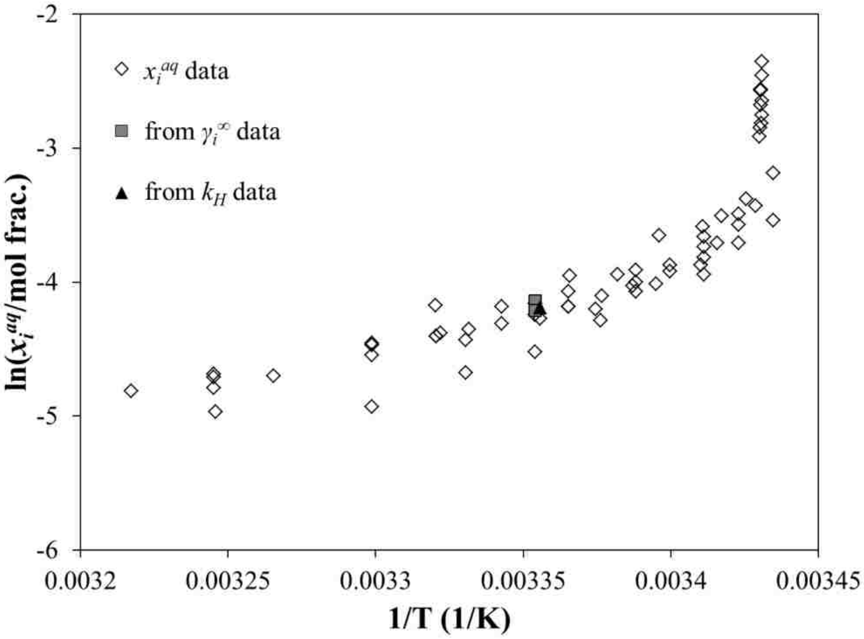

Figure 4.24: Triethylamine $x_i^{aq}$, $\gamma_i^\infty$, and $k_H$ literature data. References: [118-127]

Another example of this data analysis technique is with 2,3,4-trimethylpentane. Only $x_i^{aq}$ data are reported for this compound. Of the available $x_i^{aq}$ data, only one reference provides temperature-dependent data. However, the value at 298.15 K from the reference with temperature-dependent data does not line up with three additional references. In this instance, the three $x_i^{aq}$ values at 298.15 K that are in agreement with each other were averaged and used to derive $k_H$ and $\gamma_i^{\infty}$.

## 4.5 American Petroleum Institute Recommendations

The American Petroleum Institute (API) Technical Data Book [128] provides recommended temperature-dependent $k_H$ values for various compounds. For gases, API recommendations are based on values measured at multiple pressures. Due to the structure of the 801E database, data were entered only as a function of temperature and not pressure. Only data for gases at a pressure of 1 atm were included. The wider range of data for gases used in the API regressions renders their recommendations more reliable than what could be done in this study. In addition, the API evaluations for select liquids were determined to be reliable. As such, API recommendations for 31 compounds (26 gases and 5 liquids) were accepted in this study and are represented in the compound totals given in Table 3.2 and Table 3.3.

API temperature dependent coefficients were reported for $k_H$ in the form of DIPPR® 801 Equation 101 (see Table 4.3). Using the relationship between $k_H$ and $x_i^{aq}$ for gases leads to

$$\ln(k_H) = \ln(101.325) - \ln(x_i^{aq}) . \qquad 4.21$$

Since ln(101.325) is a constant, coefficients can be derived from the API coefficients to develop a temperature dependent equation for $x_i^{aq}$. A similar relationship was given for liquids in Equation 4.20. Since $P_i^{sat}$ is in the form of DIPPR® Equation 101 as well, the API $k_H$ and

DIPPR® 801 $P_i^{sat}$ coefficients were combined to determine $x_i^{aq}$ coefficients for liquids. Equations obtained from API equations were classified as “Derived” instead of “Smoothed”.

API regression errors are reported in various forms. The errors had to be converted to the error notation used in DIPPR® 801. If the API error was reported as an average absolute deviation (AAD) then the regression was assigned the corresponding error in the database. For example, if AAD = 5.88%, then the error reported in the database is < 10%. If the API error was reported on a log scale (i.e. standard deviation in $\ln(x_i^{aq})$ is 1.8%) then the property was calculated at $N$ points evenly distributed along the temperature range where $N$ is the number of values that were used to obtain the regression. The upper and lower uncertainty limits were calculated at these points on the normal scale, and the AAD was determined at each point. These AADs were averaged and an overall error code was assigned based on this average. The same error was assigned to $x_i^{aq}$ and $k_H$ regressions of the same compound.

API recommendations were accepted without ensuring that all of the data used in the original regression were present in the 801E database. Many of the references included in the API database were included in this study. However, the API database used high pressure data which were purposefully excluded from this study. Uncertainties of the datasets in this database were determined from the reported regression uncertainty in the same manner that uncertainties were assigned in Section 4.3.1.

### 4.6 Comparison with Literature Recommendations and Predicted Values

The temperature regressions obtained in this study were compared with available recommendations such as the IUPAC-NIST Solubility Data Series [129-165], API Technical Data Book [128], and other literature reviews. This was done to validate the evaluation procedure used in this study and to ensure that the recommended regressions of this study reflect the data included in the 801E database. Except for the API regressions mentioned in Section 4.5, outside regressions were not accepted so that a future database user can view the datasets that were used to develop the regression.

The IUPAC-NIST equation uses empirical constants that were obtained from simultaneous regression of all of the $x_i^{aq}$ data for compounds within a certain chemical family [166]. Data were then classified as "Recommended", "Tentative", "Doubtful", or "Rejected" based on the error between the regression equation and the actual literature data [150]. These classifications are given per point and not per reference; whereas, in this study, all of the points from a given reference were accepted or rejected unless there was a valid reason to split a data set (for example, the experimental method is not as accurate in a certain temperature or concentration region). In this study, temperature regressions were based solely on literature data.

If the agreement between the regressions of this study and those published was within the regression uncertainty, the parameters in this study were immediately accepted. In instances where the disagreement was larger than the regression uncertainty, the regressions were compared more judiciously. Insights gained through thermodynamic relationships, chemical family trends, and predicted values (as previously discussed) were useful in determining the best values when there were discrepancies.

In order to ensure that the analyses performed in this study were reasonable when derivative properties were excluded, recommended values determined in this study were compared to recommendations given in the literature that included derivative properties. As an example, Figure 4.25 shows methanol literature $\gamma_i^\infty$ and $k_H$ values plotted as $\ln(\gamma_i^\infty)$, the regression obtained in this study, and the regression recommended by Dohnal et al. [21]. The 95%

confidence intervals for the regression from this study are also shown. In the analysis performed by Dohnal et al. [21], the temperature-dependent parameters were obtained by simultaneously fitting $\gamma_i^{\infty}$, limiting partial molar excess enthalpy, and limiting partial molar heat capacity data. Their analysis included more properties than this study. However, their regression is within the uncertainty of the regression from this study. As an additional example, the evaluations by Plyasunov et al. [21-26] included derivative properties. Values at 298.15 K from this study were compared to their recommendations for approximately 150 compounds. The recommendations of this study are all within the reported uncertainties. These comparisons provided confidence that the properties and evaluation procedure used in this study produce reliable regressions.

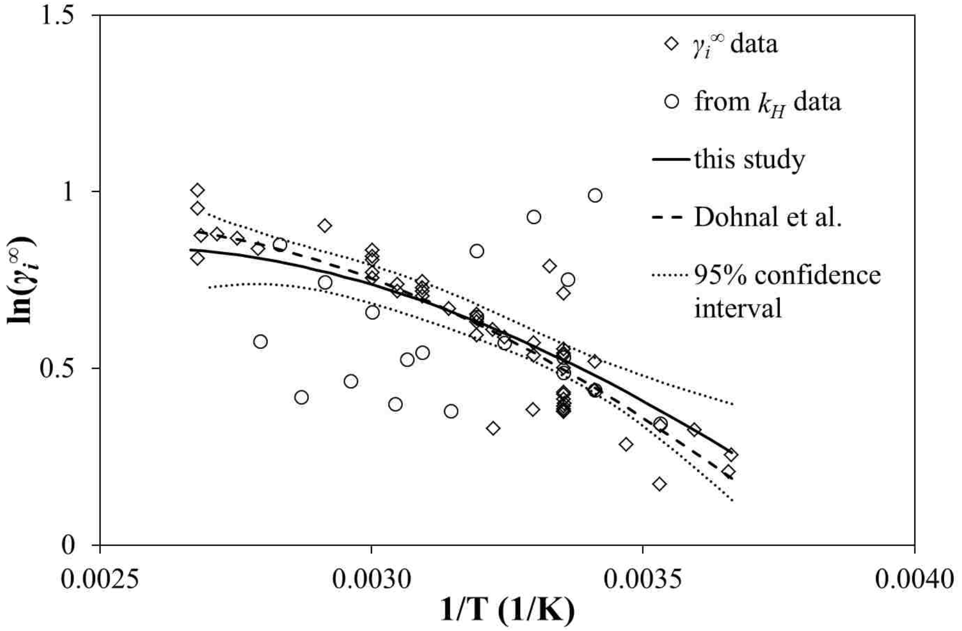

Figure 4.25: Methanol $\gamma_i^{\infty}$ regressions from this study and Dohnal et al. [21]. References: [45, 48, 69, 70, 77, 167-182]

The regressions of this study do not always match the regressions reported in the IUPAC-NIST solubility data series. Figure 4.26 shows literature $x_i^{aq}$ data for *n*-propyl formate, the regression obtained in this study, and the regression reported in the IUPAC-NIST Solubility Data Series [159]. The confidence intervals correspond to the average absolute error of the regression obtained in this study (see Section 4.3.1). In addition, the figure shows $x_i^{aq}$ data for ethyl formate for comparison purposes. The IUPAC-NIST regression extrapolates very differently from the regression in this study. However, over the temperature range of experimental data (which is the recommended range of the regression) the regressions are not statistically different. The regression of this study was accepted in the database. Similar trends were observed with additional compounds, and these compounds were handled in the same manner.

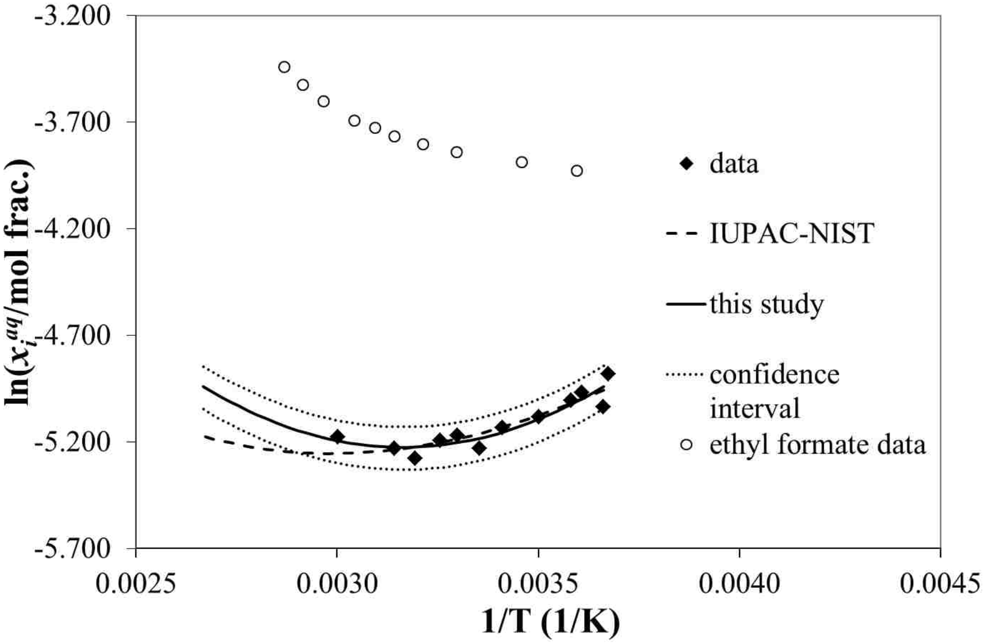

Figure 4.26: *n*-Propyl formate $x_i^{aq}$ data, regression from this study, and IUPAC-NIST [159] regression compared to ethyl formate $x_i^{aq}$ data. References: [183, 184]

Figure 4.27 is an example that shows how data from the combined properties help in the data analysis process. The $x_i^{aq}$ data for di-*n*-propyl ether are shown along with $x_i^{aq}$ values calculated from literature $k_H$ and $\gamma_i^{\infty}$ data. All of the $x_i^{aq}$ data were reported in the same paper, but two experimental methods were used. The $x_i^{aq}$ dataset that does not agree with the $k_H$ and $\gamma_i^{\infty}$ data were measured using a less reliable method, so those points were rejected. The $k_H$, $\gamma_i^{\infty}$, and remaining $x_i^{aq}$ data were used to obtain the regression shown in the plot. The IUPAC-NIST [158] trend is also shown, and it is significantly different over the entire temperature range. All of the IUPAC-NIST ether trends use theoretical coefficients, and all ether systems (except one) are forced to exhibit a minimum at 360 K [185]. The regression of this study is recommended because it matches experimental data from multiple references and properties.

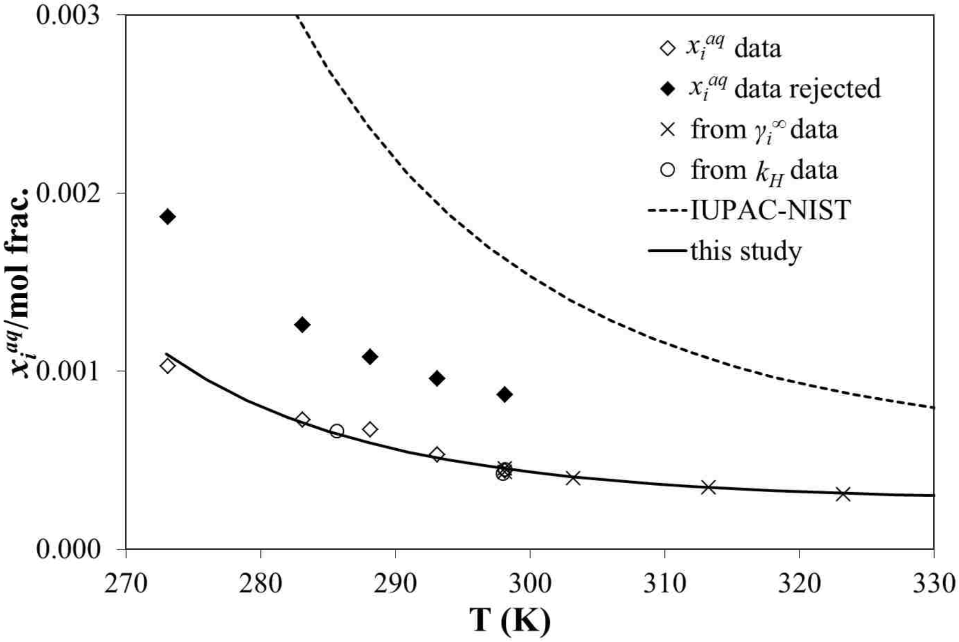

Figure 4.27: di-*n*-Propyl ether $x_i^{aq}$ regressions from this study and from IUPAC-NIST [158]. References: [47, 172, 186-189]

Another example is shown below (Figure 4.28) where the regressions are significantly different over part of the data range. The figure shows literature $x_i^{aq}$ data for 3-methyl-3-pentanol, the regression obtained in this study with the average confidence intervals, and the regression reported in the IUPAC-NIST Solubility Data Series [150]. Some of the data were rejected because the data are old (measured in 1938), and the experimental and analytical methods used are not as reliable as the methods used with the more recent data. The IUPAC-NIST regression shows significantly different behavior as temperature increases. The regression from this study was accepted because it follows the available experimental data.

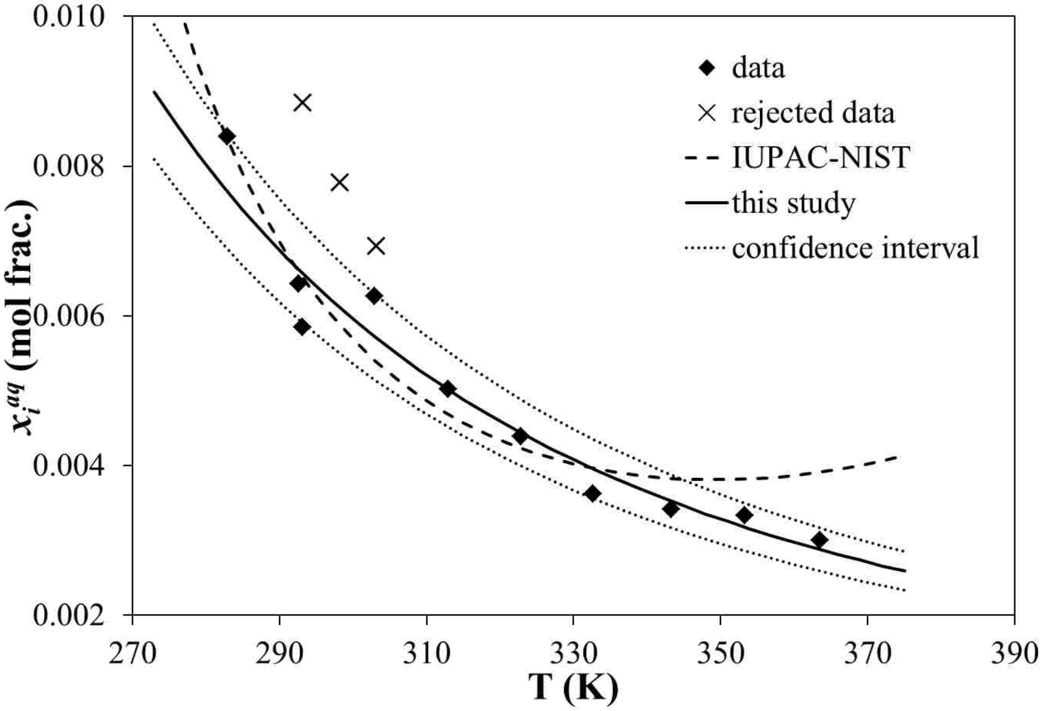

Figure 4.28: 3-Methyl-3-pentanol $x_i^{aq}$ regressions from this study and from IUPAC-NIST [150]. References: [44, 190]

In the following examples, $k_H$ values predicted using the group contribution method of Sedlbauer et al. [191] were used to help identify the best datasets. The Sedlbauer et al. [191] method was developed using data for multiple hydrocarbons, so it can be used reliably to identify the best datasets for similar types of compounds. Values were converted between $x_i^{aq}$ and $k_H$ using Equation 4.1 and DIPPR® 801 [117] $P_i^{sat}$ data.

When the data evaulation methods already discussed were not helpful in distinguishing between conflicting data sets for a compound, prediction methods (discussed in Chapter 7) were helpful in identifying the best datasets. As an example, with cumene there are multiple $x_i^{aq}$ temperature trends shown by literature data (Figure 4.29). More data are available in the literature for this compound than are shown in the figure; however, there is enough scatter in these additional data that they do not aid in identifying the best trend. These additional datasets were included in data analysis, but they are not shown in the figure for viewing purposes. The predicted Sedlbauer et. al [191] values ($k_H$ converted to $x_i^{aq}$) and IUPAC-NIST [136] curve are the closest to the data from reference b [192] while the API [128] regression is based on the data of reference c [193]. The IUPAC-NIST [136] trend is based on $x_i^{aq}$ data for multiple hydrocarbons. The prediction method of Sedlbauer et al. [191] was developed using data for multiple aromatic hydrocarbons, so the trend inherently takes into account chemical family trends. The relative agreement between the Sedlbauer et al. [191] and IUPAC-NIST [136] recommendations is encouraging because both used information gained from examining multiple compounds with similar structures. Because of this, the data from reference b [192] are recommended.

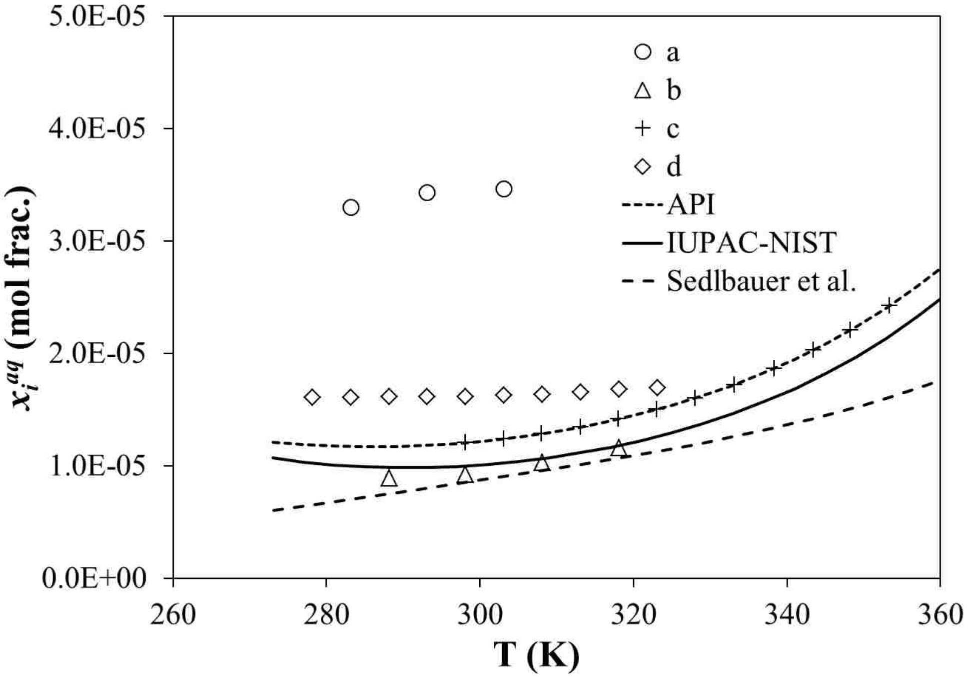

Figure 4.29: Cumene $x_i^{aq}$ data compared with Sedlbauer et. al [191] predicted values and API [128] and IUPAC-NIST [136] recommendations. References: a [194], b [192], c [193], d [105]

As another example, limited data are available for 2,2,5-trimethylhexane. The available literature $x_i^{aq}$ values are plotted as $\ln(k_H)$ versus inverse temperature in Figure 4.30 with $k_H$ values predicted using the group contribution method developed by Sedlbauer et al. [191]. Data for this compound were not included in the Sedlbauer et al. [191] method development; however, data for other aliphatic hydrocarbons were included making the method applicable for this compound. The difference between the two reported values at 298.15 K (0.00335 $K^{-1}$ on the inverse temperature scale) make it difficult to identify the best values by looking at the data alone. The predicted values are in agreement with the data points reported by reference a [195], so these values were accepted.

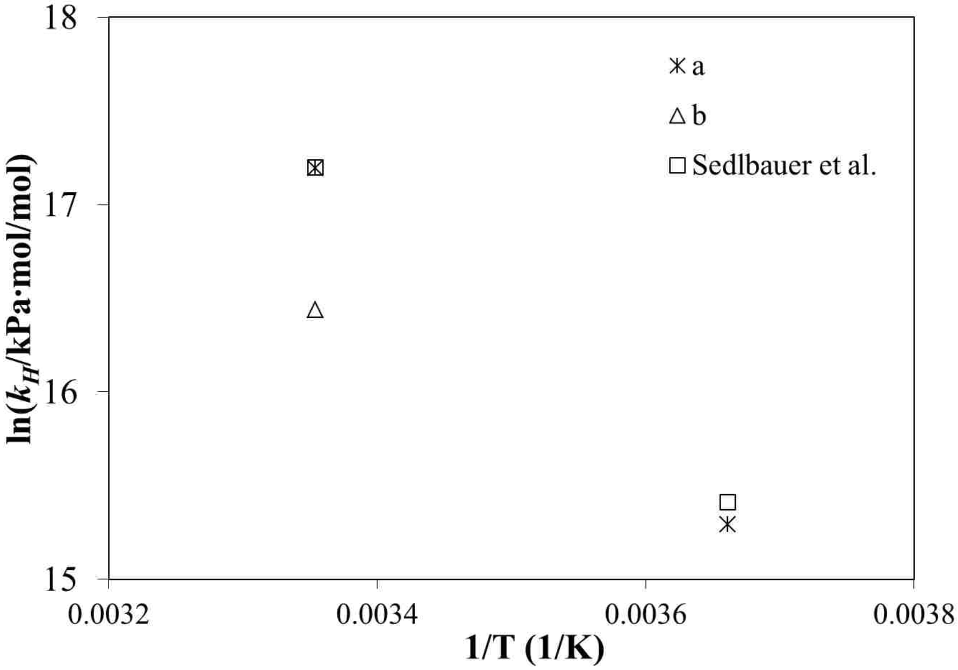

Figure 4.30: 2,2,5-Trimethylhexane $x_i^{aq}$ data plotted as ln($k_H$) compared with Sedlbauer et. al [191] predicted values. References: a [195], b [86]

## 4.7 Summary

A database containing recommended values for $k_H$, $\gamma_i^\infty$ and $x_i^{aq}$ of industrially important chemicals has been compiled for aqueous systems. Recommendations have been provided for at least one of these properties for 509 compounds. The structure of this database is compatible with the existing DIPPR® 801 database and DIADEM interface. Thermodynamic relationships, chemical family trends, and predicted values were important data analysis tools. Data from the various properties were related to each other using thermodynamic relationships and reliable DIPPR® 801 pure component property values. For hydrophobic compounds, the data from the three properties were combined to obtain recommendations. In instances where the data could not be combined, the thermodynamic relationships were helpful in identifying the best datasets.

Chemical family plots were used with temperature-dependent and single-temperature data to check for consistency within chemical families and to select the best data. Predicted values were used to select the best datasets when there were discrepancies in the literature data. Notes in the database provide information about the procedure and data used to provide recommendations for each compound and property.

# 5 Experimental Methods

The inert gas stripping (IGS) method has been used to measure both $k_H$s and $\gamma_i^\infty$s [37, 196]. In this study, $k_H$s and $\gamma_i^\infty$s were measured for various compounds at temperatures between 8°C and 50°C using the IGS method. Compounds in this study were selected based on the absence of experimental data or inconsistencies between reported experimental values. Some of the inconsistencies occur between experimentally determined $k_H$s and calculated $k_H$s (Equation 4.1).

## 5.1 Materials

The compounds used as solutes are listed in Table 5.1 with the suppliers and stated purities. Chemicals were used as received without further purification. Deionized distilled water was used as the solvent.

Table 5.1: Compounds and purities

| Chemical | CAS | Supplier | Purity |
|---|---|---|---|
| Toluene | 108-88-3 | Sigma-Aldrich | 99.8% |
| 1-Butanol | 71-36-3 | Macron Chemicals | ≥99.4% |
| Anisole | 100-66-3 | Sigma-Aldrich | ≥99.0% |
| 1,2,3-Trichlorobenzene | 87-61-6 | Sigma-Aldrich | 99% |
| 1,2-Difluorobenzene | 367-11-3 | Sigma-Aldrich | 98% |
| 4-Bromotoluene | 106-38-7 | Sigma-Aldrich | 98% |
| 2,4-Dichlorotoluene | 95-73-8 | Sigma-Aldrich | 99% |

## 5.2 Inert Gas Stripping Theory

The IGS method uses gas chromatography (GC) to analyze the change in composition with time of the vapor phase produced from stripping a dilute solution. The IGS methods of Leroi et al. (1977) and Mackay et al. (1979) were developed separately for $\gamma_i^\infty$ and $k_H$, respectively [37, 196]; however, the experimental methods are the same and were derived using the same equations and assumptions. Mackay's method uses the relationship between $k_H$ and $\gamma_i^\infty$ (Equation 4.3). The equation developed by Leroi has been expanded by multiple authors [197-199], but an analogous expansion has not been reported for $k_H$. The following is the theory behind the IGS method as described by Krummen et al. [198]. The equations have also been written in terms of $k_H$ in this study to easily apply them to solid solutes.

In vapor-liquid equilibrium, the following is used to describe the solute

$$y_i \hat{\phi}_i^V P = \gamma_i x_i f_i^L , \tag{5.1}$$

where $y_i$ is the mole fraction in the vapor phase, $\hat{\phi}_i^V$ is the partial molar fugacity coefficient of species $i$ in the vapor phase, $P$ is the total pressure, $\gamma_i$ is the activity coefficient relative to the pure-component standard state, $x_i$ is the mole fraction in the liquid phase, and $f_i^L$ is the fugacity of pure species $i$ in the liquid phase. In this study, it was assumed that $\hat{\phi}_i^V = 1$. Since the solute concentration is very small, $\gamma_i$ can be replaced by $\gamma_i^\infty$.

For liquids, the liquid fugacity of pure species $i$ is calculated at the system temperature using

$$f_i^L = \phi_i^{sat} P_i^{sat} , \tag{5.2}$$

where $P_i^{sat}$ is the vapor pressure and $\phi_i^{sat}$ is the vapor-phase fugacity coefficient of pure species $i$ at its saturation pressure. This equation assumes the Poynting factor is unity which is valid at atmospheric pressure. Substituting Equation 5.2 into 5.1 gives

$$y_i P = x_i \gamma_i^{\infty} \phi_i^{sat} P_i^{sat} . \tag{5.3}$$

The vapor-liquid equilibrium can be written in terms of $k_H$ by substituting Equation 4.2 into 5.1 which results in Equation 2.3 given in Section 2.1.3 :

$$y_i P = x_i k_H . \tag{2.3}$$

This relationship can be used for liquid and solid solutes. The solvent can be described by

$$y_{solv} P = P_{solv}^{sat} , \tag{5.4}$$

where $y_{solv}$ is the mole fraction of water in the vapor phase and $P_{solv}{}^{sat}$ is the solvent vapor pressure. This equation assumes that the Poynting factor and vapor-phase corrections are negligible and that the activity coefficient of solvent is unity which is valid because $x_{solv} \approx 1$.

The equations used to determine $k_H$ and $\gamma_i^{\infty}$ using the IGS method are based on mass balances around the system. The mass balance assumes that only solute is stripped from the stripping cell which is accomplished by saturating the stripping gas with solvent before it enters the stripping cell. Additionally, these balances assume ideal gas behavior (valid since experiments were conducted at atmospheric pressure), negligible dissolution of the carrier gas in the system, additive gas volumes (valid at constant temperatures and pressures in unreactive systems), and small concentrations of solute in the headspace ($y_i \approx 0$). Figure 5.1 depicts the inlets and outlets to the cells used in the mass balances.

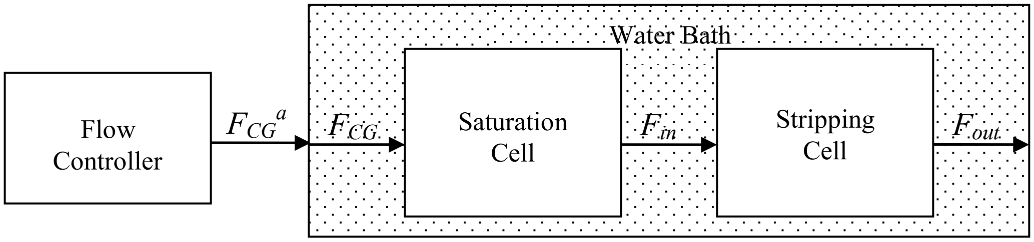

Figure 5.1: Inlets and outlets of saturation and stripping cells used in mass balances

The flow rate of carrier gas entering the saturation cell ($F_{CG}$) is determined from the measured volumetric flow rate at ambient conditions ($F_{CG}{}^a$), cell temperature ($T$), and ambient temperature ($T^a$) using

$$F_{CG} = F_{CG}^a \cdot \frac{T}{T^a}. \qquad 5.5$$

The volumetric flow rate entering the stripping cell ($F_{in}$) is equal to the sum of the carrier gas flow rate and the flow rate due to solvent saturation ($F_{solv}$):

$$F_{in} = F_{CG} + F_{solv}. \qquad 5.6$$

The flow rate of solvent leaving the saturation cell and entering the stripping cell is described by

$$F_{solv} = F_{in} y_{solv} = F_{in} \frac{P_{solv}^{sat}}{P}. \qquad 5.7$$

Krummen et al. [198] use $F_{CG}$ instead of $F_{in}$ in Equation 5.7 which is incorrect. Combining Equations 5.6 and 5.7 and rearranging to solve for $F_{in}$ yields

$$F_{in} = \frac{F_{CG}}{\left(1 - \frac{P_{solv}^{sat}}{P}\right)}. \qquad 5.8$$

The flow rate leaving the stripping cell is the sum of the flow entering the cell and the flow rate of stripped solute ($F_i$):

$$F_{out} = F_{in} + F_i . \qquad 5.9$$

Using an Equation analogous to 5.7 for the stripping cell yields

$$F_i = F_{out} y_i , \qquad 5.10$$

where $y_i$ is the mole fraction of solute exiting the stripping cell. This assumes that only solute is stripped from the stripping cell (accomplished by first saturating the carrier gas with solvent) and ideal gas behavior. Combining 5.9 and 5.10 and solving for $F_{out}$ yields

$$F_{out} = \frac{F_{in}}{1 - y_i} . \qquad 5.11$$

$F_i$ can also be described by

$$F_i = -\frac{RT}{P}\frac{dn_i}{dt} , \qquad 5.12$$

where $n_i$ is the moles of solute in the stripping cell which changes with time ($t$) and $R$ is the universal gas constant. The derivative term is determined assuming ideal gas behavior:

$$\frac{dn_i}{dt} = -y_i \frac{PF_{out}}{RT} . \qquad 5.13$$

Substituting Equation 5.11 into 5.13 and using the phase equilibrium equation for $y_i$ obtained from Equation 5.3 yields

$$\frac{dn_i}{dt} = -x_i \gamma_i^{\infty} \phi_i^{sat} P_i^{sat} \frac{1}{RT} \frac{F_{in}}{1 - \frac{x_i \gamma_i^{\infty} \phi_i^{sat} P_i^{sat}}{P}} . \qquad 5.14$$

The total moles of solute in the stripping cell is the sum of the moles of solute in the liquid (*L*) and vapor (*V*) phases:

$$n_i = n_i^L + n_i^V \; . \tag{5.15}$$

Assuming that the total number of moles in the cell is equal to the number of moles of solvent in the cell (which is valid since $n_{solv} >> n_i$) and assuming that the vapor phase can be described by an ideal gas yields:

$$n_i = x_i n_{solv} + y_i \frac{PV_g}{RT}, \tag{5.16}$$

where $V_g$ is the volume of the headspace in the stripping cell. The total cell volume was determined by filling the cell completely with water and measuring the mass, and then calculating volume using water density. The volume of water added to the cell for each experiment (calculated from the known mass and density) was subtracted from the total cell volume to obtain $V_g$. Substituting Equation 5.3 into 5.16 and rearranging results in an equation for $x_i$:

$$x_i = \frac{n_i}{n_{solv} + \gamma_i^{\infty} \phi_i^{sat} P_i^{sat} \dfrac{V_g}{RT}} \; . \tag{5.17}$$

Combining 5.14 and 5.17 yields:

$$\frac{dn_i}{dt} = -x_i \gamma_i^{\infty} \phi_i^{sat} P_i^{sat} \frac{1}{RT} \frac{F_{in}}{1 - \dfrac{\gamma_i^{\infty} \phi_i^{sat} P_i^{sat}}{P} \cdot \dfrac{n_i}{n_{solv} + \gamma_i^{\infty} \phi_i^{sat} P_i^{sat} \dfrac{V_g}{RT}}} \; . \tag{5.18}$$

In this study it was assumed $y_i << 1$ so that

$$\frac{1}{1-y_i} \approx 1. \tag{5.19}$$

With this assumption, 5.18 simplifies to

$$\frac{dn_i}{dt} = -\frac{n_i}{n_{solv} + \gamma_i^\infty \phi_i^{sat} P_i^{sat} \frac{V_g}{RT}} \gamma_i^\infty \phi_i^{sat} P_i^{sat} \frac{F_{in}}{RT}. \tag{5.20}$$

The only variable that is a function of time is $n_i$. Integration yields

$$\ln\left(\frac{n_i}{n_i^0}\right) = -\frac{\gamma_i^\infty \phi_i^{sat} P_i^{sat}}{n_{solv} + \gamma_i^\infty \phi_i^{sat} P_i^{sat} \frac{V_g}{RT}} \frac{F_{in}}{RT} t, \tag{5.21}$$

where the superscript *0* indicates the initial condition. Assuming that concentration is proportional to GC peak area (*A*) gives:

$$\ln\left(\frac{A}{A^0}\right) = -\frac{\gamma_i^\infty \phi_i^{sat} P_i^{sat}}{n_{solv} + \gamma_i^\infty \phi_i^{sat} P_i^{sat} \frac{V_g}{RT}} \frac{F_{in}}{RT} t. \tag{5.22}$$

A plot of $\ln(A/A^0)$ versus *t* yields a straight line with slope, *a*:

$$a = \frac{\ln\left(\frac{A}{A^0}\right)}{t}. \tag{5.23}$$

Substituting 5.23 into 5.22 and rearranging gives:

$$\gamma_i^\infty = \frac{-RTn_{solv}}{\phi_i^{sat} P_i^{sat} \left( V_g + \frac{F_{CG}}{\left(1 - \frac{P_{solv}^{sat}}{P}\right) a} \right)}. \tag{5.24}$$

This equation is slightly different from that reported by Krummen et al. [198] due to the change in Equation 5.7. Equation 5.24 refers specifically to liquid solutes where the liquid fugacity of the pure species can be calculated using Equation 5.2. Using Equation 2.3 to describe the phase equilibrium and the methodology outlined above results in an equation for $k_H$:

$$k_H = \frac{-RTn_{solv}}{V_g + \dfrac{F_{CG}}{\left(1 - \dfrac{P_{solv}^{sat}}{P}\right)a}}. \qquad 5.25$$

In order to determine $\phi_i^{sat}$, the virial equation truncated after the second virial coefficient, $B$, was used,

$$Z = \frac{PV}{RT} = 1 + \frac{BP}{RT}, \qquad 5.26$$

where $Z$ is the compressibility factor and $V$ is volume.

At a constant temperature, $\phi_i^{sat}$ is determined by:

$$\ln \phi_i^{sat} = \int_0^{P_i^{sat}} \left(Z_i^V - 1\right)\frac{dP}{P}. \qquad 5.27$$

Using 5.26 results in:

$$\phi_i^{sat} = \exp\left(\frac{B_{ii}P_i^{sat}}{RT}\right). \qquad 5.28$$

Temperature dependent equations for $B_{ii}$ were obtained from the DIPPR® 801database[117]. In instances where data were not available within the experimental temperature range, $\phi_i^{sat}$ was assumed to be unity. For compounds that were solids, Ψ was used to calculate $\gamma_i^{\infty}$ as outlined in Section 4.1.

## 5.3 Apparatus and Procedure

Dilute solutions (on the order of $10^{-3}$ mole fraction or less) of each of the individual compounds listed in Table 5.1 were made in a glass cell with a diameter of 5 cm and total volume of 414 mL. Literature $x_i^{aq}$ values were referenced to ensure the concentration in the cell was below the solubility limits for the compound in question. The solution was allowed to mix for several hours, typically overnight, to ensure equilibrium was reached. A similar glass cell was filled with deionized, distilled water and was used as the saturation cell. Both cells were threaded and sealed with threaded Teflon caps and Viton or Kalrez o-rings. All the fittings (316 stainless steel) were threaded into the Teflon lid to ensure a leak tight fit. Swagelok® quick-connects allowed easy removal of both cells from the system for cleaning purposes. The temperature of the stripping cell was measured using an RTD digital thermometer (Omega, Model HH804) while the pressure was measured using a pressure transducer (Paroscientific, Model 740). Cell pressure varied slightly from ambient pressure with higher flow rates.

Nitrogen (≥99.998%) was used as the carrier gas. The flow rate was controlled by a mass flow controller (Aalborg, GFC17). Two controllers were used with ranges of 0-12 and 0-200 mL/min and accuracies of ±1.5%FS. Nitrogen was first bubbled through the saturation cell that contained only water. The saturated nitrogen was then bubbled through the dilute solution in the stripping cell. Small bubbles were formed in both cells using a 2 μm porous 316L stainless steel filter element (Mott). The stripping cell was continuously mixed with a magnetic Teflon stir bar. Both cells were in a water bath controlled by a temperature controller (Omega, CSi32). At temperatures of 298.15 K or below, a cooling loop (Neslab, RTE-8DD) was used in addition to the heating element for temperature control. The temperature of the bath was periodically checked using a mercury-in-glass thermometers (scale of 0.1 K), and it stayed within ±0.1 K of the set point.

Gas exiting the stripping cell entered a transfer line that was heated to 403.15 K using a fiberglass heating cord (Omega, #HTC-120) to prevent condensation in the transfer line. The transfer line was made of 1/8” (3.175 mm) 304 stainless steel tubing and was wrapped in aluminum, the heating cord, and then fiber glass insulation. Transfer line temperature was measured and controlled using a type-K thermocouple and temperature controller (Omega, Model CN7500). The transfer line was connected to the gas sampling valve of a GC (Agilent, 7890A) equipped with a flame ionization detector (FID). Helium (≥99.995%) was used as the GC carrier gas. Hydrogen (≥99.95%) and ultra zero air were used with the FID. An Equity-5 column (Supelco, #28089-U) was installed in the GC. A schematic of the apparatus is given in Figure 5.2.

In order to develop the GC methods, dilute solutions of each compound were made in test tubes. An additional solution was made that also contained acetone. Acetone was used to clean the cells between experiments. In many experiments, trace amounts of acetone were present despite efforts to remove it during the cleaning process (described later in this section). Manual liquid injections were performed using both solutions to develop the methods. Conditions were changed in order to elute sharp peaks and optimize the separation between acetone and the compound of interest. The method had to separate the compound and acetone peaks to eliminate any potential interference. The GC conditions used throughout experimentation that were the same for every method are listed in Table 5.2. The conditions that were changed for each compound are listed in Table 5.3.

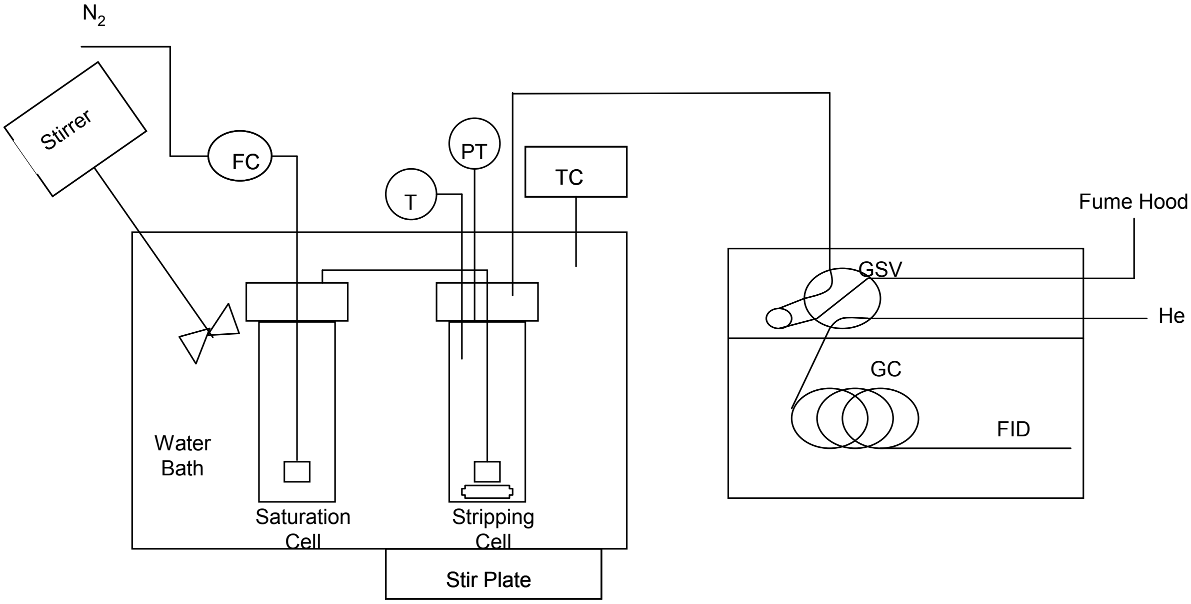

Figure 5.2: IGS apparatus

Table 5.2: Constant GC conditions

| Component | Conditions |
|---|---|
| GSV | 130°C |
| FID | $H_2$: 40 mL/min<br>Air: 450 mL/min<br>Makeup He: 25.388 mL/min |

Table 5.3: GC conditions for each compound

| Compound | Inlet | FID | Oven Temperature Program |
|---|---|---|---|
| Toluene | 130°C<br>Split ratio: 100 | 250°C | 130°C for 0.5 min; ramp at rate of 20°C/min up to 175°C; hold 1 min |
| 1-Butanol | 130°C<br>Split ratio: 100 | 250°C | 100°C for 0.5 min; ramp at rate of 15°C/min up to 140°C |
| 4-Bromotoluene | 100°C<br>Split ratio: 100 | 250°C | 100°C for 0.5 min; ramp at rate of 10°C/min up to 120°C; hold 0.1 min |
| Anisole | 155°C<br>Split ratio: 100 | 275°C | 150°C for 0.5 min; ramp at rate of 10°C/min up to 165°C; hold 1.5 min |
| 1,2,3-Trichlorobenzene | 130°C<br>Split ratio: 40 | 275°C | 200°C for 0.5 min; ramp at rate of 20°C/min up to 250°C; hold 0.1min |
| 2,4-Dichlorotoluene | 130°C<br>Split ratio: 100 | 275°C | 185°C for 0.5 min; ramp at rate of 10°C/min up to 208°C |

Since relative concentrations are required instead of actual concentrations, each stripping cell was used for multiple experiments. Initially, one temperature was chosen and the flow rate was changed in a randomized order to determine an optimal flow rate for the experiments over the temperature range of interest. It was assumed that equilibrium would be attained at the other temperatures because a conservative flow rate was chosen. Once the flow rate was selected, the experimental temperature was randomized in measuring the determined number of replicates at each temperature. The amount of time required between runs with the same cell varied depending on the variables that were changed. If temperature was changed, the cell was allowed to mix for at least 30 minutes once it reached the new temperature set point. In addition, the transfer line was flushed between runs to remove any chemical from the previous experiment.

When experiments were completed with a given stripping cell, the cell was thoroughly cleaned before the next experiment. After proper disposal of the aqueous waste, the stripping cell and frit were rinsed with acetone to remove any residual chemical before the cell was washed in the sink since some of the chemicals used are potentially harmful to the environment. Everything was then washed off with soapy water and rinsed with water. A minimum of 30 mL of acetone was then forced through the frit using a syringe. All of the cell components (including all stainless steel tubing) were then rinsed again with acetone. About 100 mL of deionized water was then forced through the frit using a syringe in an effort to remove the acetone. All cell components were then given a final rinse with deionized water and allowed to dry completely before a new cell was prepared. $N_2$ was used to speed up the drying process of the frit and portions of the tubing. The saturation cell was cleaned in a similar manner. It was not cleaned as often since the only compound entering the cell was $N_2$. The saturation cell did not have to dry completely before it was used since it was unnecessary to know the amount of water in the cell.

# 6 Experimental Results and Discussion

The apparatus was first validated by measuring the $k_H$s and $\gamma_i^\infty$s of toluene and 1-butanol at various temperatures. Table 6.1 compares the values obtained in this study with literature values. The percent standard deviations of the average $k_H$ values ($s_{kH}$) and corresponding $\gamma_i^\infty$ values ($s_{\gamma\infty}$) are included in addition to the number of measurements, $N$. Also given are the 95% confidence intervals (CIs) of the average $k_H$ calculated using a Student's T distribution. The CIs are reported as a percentage of the average. CIs cannot be calculated using a Student's T distribution when $N = 1$. The reported $\gamma_i^\infty$ standard deviations, $s_{\gamma\infty}$, were determined using the $s_{kH}$ values and propagation of error. In cases where only one measurement was performed, the reported $s$ is an estimated uncertainty. Literature values calculated from $\gamma_i^\infty$ and $P_i^{sat}$ are noted in the table. There have been reported problems with using IGS to measure $k_H$s of *n*-alkanols (including 1-butanol) [68]. Reported *n*-alcohol values using IGS are higher than values measured using a static equilibration method, and this difference has been attributed to evaporation in the stripping cell and adsorption to the bubble surface. However, the values obtained in this study are comparable to other literature values. The largest discrepancy is at the lowest temperature measured. This corresponds to a low $k_H$ meaning it was more difficult to measure a change in concentration with time. The use of toluene and 1-butanol to validate the method established a broad range of $k_H$s for which this method is applicable.

For each compound, multiple flow rates were tested to ensure equilibrium was reached because the measured $k_H$ should not be a function of flow rate if the system is at equilibrium. If the flow rate was too high, $k_H$ would appear lower because there was not as much time for the bubbles to equilibrate with the solution resulting in a lower concentration of solute in the bubble. Problems were also observed if the flow rate was too small. For compounds with lower $k_H$ values, if the flow rate was too small, it was difficult to detect a change in concentration with time which resulted in noisy GC data. Table 6.2 gives the flow rates that were tested for each compound and the temperature of the flow rate experiments. Equilibrium was reached at flow rates that resulted in $k_H$ values that were not statistically different (analysis of variance p-values > 0.05). The bolded values are the flow rates that were selected for subsequent experiments at other temperatures. The flow rates that resulted in lower $k_H$ values are also listed. For toluene, 4-bromotoluene, and 2,4-dichlorotoluene, all of the flow rates tested resulted in equilibrium. For anisole and 1,2,3-trichlorobenzene, flow rates were tested at multiple temperatures due to the noise in the GC data at some of the flow rates. Higher flow rates typically resulted in higher $R^2$ values, but equilibrium was not always reached.

Table 6.1: Toluene and 1-butanol results at ambient pressure (approximately 12.5 psia) from this study and literature

| $T$/K | $k_H$ /kPa | $s_{kH}$ /% | $N$ | CI/% α=0.05 | Lit. $k_H$/kPa | $\phi_i^{sat}$ | $\gamma_i^\infty$ | $s_{\gamma\infty}$/% | Lit. $\gamma_i^\infty$ |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | Toluene | | | | |
| 298.15 | $3.35\cdot10^4$ | 12 | 13 | 7 | $3.69\cdot10^4$ [192] | 0.996 | $8.84\cdot10^3$ | 13 | $9.20\cdot10^3$ [200] |
| 308.15 | $5.46\cdot10^4$ | 5.2 | 2 | 47 | $5.44\cdot10^4$ [201][a] | 0.994 | $8.81\cdot10^3$ | 7.3 | $8.72\cdot10^3$ [200] |
| | | | | | 1-Butanol | | | | |
| 298.15 | 69.4 | 8.0 | 1 | NA | 49.4 [202] | 0.996 | 77.4 | 26 | 48.4 [168] |
| 308.15 | 105 | 4.1 | 1 | NA | 115 [203] | 0.995 | 58.9 | 26 | 57.2 [168] |
| 313.15 | 140 | 4.3 | 1 | NA | 123 [180][a]<br>146 [168][a] | 0.993 | 56.5 | 26 | 49.5 [180]<br>58.9 [168] |
| 323.15 | 261 | 10 | 2 | 92 | 274 [204] | 0.991 | 57.5 | 27 | 59.4 [168] |

[a] from $\gamma_i^\infty \cdot P_i^{sat}$

Table 6.2: Flow rates tested and used in this study

| Compound | Flow Rates Resulting in Equilibrium (mL/min) | Flow Rates Not Resulting in Equilibrium (mL/min) | *T*/K |
|---|---|---|---|
| Toluene | 12, **40**, 75 | NA | 298.15 |
| 1-Butanol | 200 | Data too noisy at lower flow rates | 298.15 |
| Anisole | 125, **160** | 200 | 281.02 & 293.15 |
| 1,2-Difluorobenzene | 20, **40** | 12, 60, 80 | 298.22 |
| 4-Bromotoluene | 20, **40**, 60, 80 | NA | 308.10 |
| 1,2,3-Trichlorobenzene | **20**<br>**20, 40**<br>**40, 60** | 40, 60<br>60, 80<br>NA | 281.01<br>293.07<br>322.93 |
| 2,4-Dichlorotoluene | 20, **40**, **60**, 80 | NA | 293.09 |

During the method validation process, it was discovered that allowing the frit to soak overnight in the solution resulted in small bubbles (diameter < 1 mm). If the frit is not completely wetted, then there are a small number of paths with less resistance where all of the nitrogen exits resulting in larger bubbles (diameter > 1 mm). In the instances of larger bubbles, the measured $k_H$ values were low because of mass transfer limitations to the equilibration. The solutions were made the night before to allow the frit to soak and to ensure complete mixing. To ensure that the mixing time did not result in erroneous values due to adsorption effects, the equilibration time was varied from 3 hours to 2 days for 1,2-difluorobenzene. There was no difference within the results, so adsorption effects in the cell due to equilibration time were determined to be negligible. Periodically the cells were bypassed allowing only nitrogen to go through the transfer line to ensure there was no chemical holdup in the line. The GC analysis from these trials confirmed there was no holdup.

Using the $k_H$ values obtained in this study and Equation 2.3, values of $y_i$ were calculated based on experimental conditions to determine the validity of the assumption that $y_i \approx 0$ used in the IGS theory. Table 6.3 lists the maximum $y_i$ values that were encountered at any time during any of the runs for each compound. The most significant $y_i$ is from the 1,2-difluorobenzene experiments. However, this contribution was still considered negligible. Since the cells were used for multiple, randomized experiments, the majority of the runs associated with a given temperature had a much lower initial concentration. There was not a statistically significant difference between the $k_H$ values from the experiment with the starting concentration listed in Table 6.3 and the experiments that had smaller starting concentrations. The $k_H$ values from runs that started at a more dilute condition were not statistically different from those that started at higher concentrations.

Table 6.3: Maximum headspace concentrations possible in this study

| Compound | Max $y_i$ (mole fraction) |
|---|---|
| Toluene | $3.09 \cdot 10^{-2}$ |
| 1-Butanol | $2.86 \cdot 10^{-3}$ |
| Anisole | $1.06 \cdot 10^{-2}$ |
| 1,2-Difluorobenzene | $1.08 \cdot 10^{-1}$ |
| 4-Bromotoluene | $2.19 \cdot 10^{-3}$ |
| 1,2,3-Trichlorobenzene | $1.46 \cdot 10^{-4}$ |
| 2,4-Dichlorotoluene | $3.05 \cdot 10^{-3}$ |

Solutions of varying concentrations of both 1,2-difluorobenzene and toluene were made in order to verify the linearity of the detector (FID). A linear response was observed for both compounds. Peak areas for the vapor samples observed during experimentation fell within the peak areas of the liquid samples used to check linearity. For the other compounds, it was assumed that the detector response was linear because small concentrations were used.

During the experiments, it was observed that adsorption effects in the apparatus became significant after the concentration in the cell dropped below a lower limit. A wide range of $k_H$

values were obtained for the same compound at the same temperature and flow rate even though the plots of $\ln(A/A^0)$ versus time had $R^2$ values greater than 0.99. Plots were made of the slope (Equation 5.23) as a function of time to determine how the cumulative slope changed with the addition of a new point. In some cases, the slope equilibrated to a constant value whereas in other instances it never settled as illustrated with 1,2-difluorobenzene data in Figure 6.1 and Figure 6.2. Figure 6.1 shows GC data from two separate experiments at the same conditions. Both experiments resulted in high $R^2$ values (>0.99); however, they gave different slopes resulting in significantly different $k_H$ values. Figure 6.2 shows the change of slope with time for the GC data shown in Figure 6.1. The cumulative slope of Run A never settled to a constant value. In all instances where the slope continued to change with time for each compound, the $k_H$ values were lower than when the slope reached a constant value. The changing slope only occurred when the peak areas (solute concentration) dropped below a value that was compound dependent. It is suspected that adsorption effects in the cell became significant once the solution concentration dropped below a certain value. Since calibration is not required for this method, the exact lower limit concentrations were not determined. The lower limit was estimated to be below 1% of the solubility limit with 1,2-difluorobenzene. The plots of the cumulative slope versus time allowed determination of when this lower limit was passed for each compound. Data were not used to deter mine $k_H$ values from any experiments where adsorption was significant.

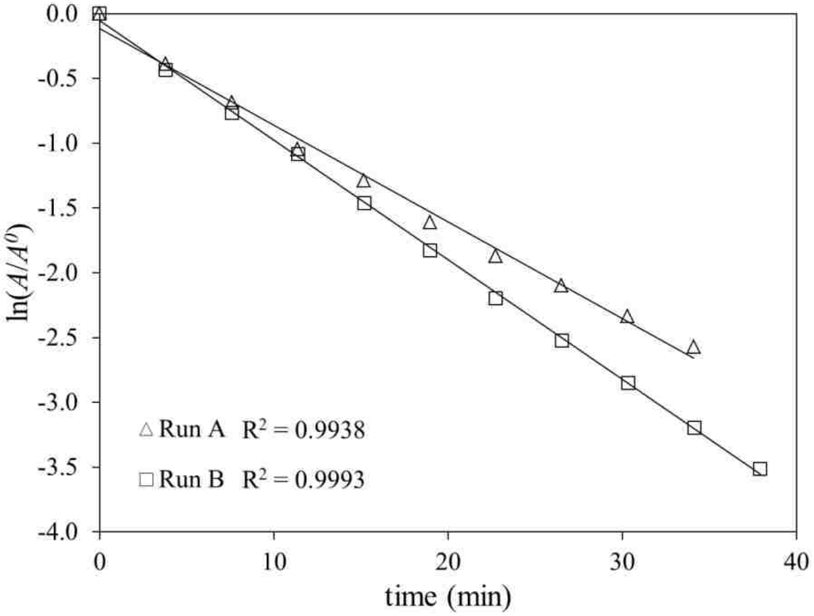

Figure 6.1: GC data for two separate 1,2-difluorobenzene experiments at 323.15 K and a $N_2$ flow rate of 40 mL/min that resulted in different slopes (*a*)

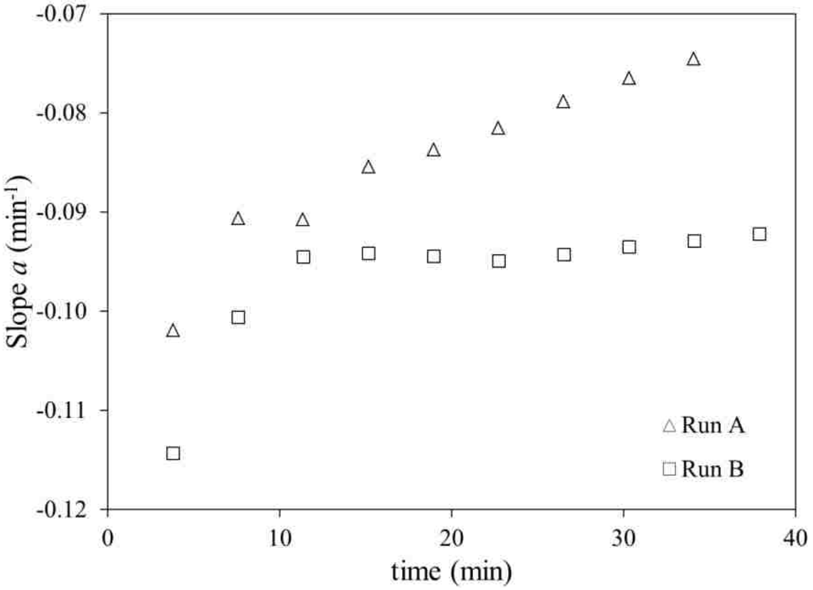

Figure 6.2: Cumulative slopes (*a)* from GC data shown in Figure 6.1 as a function of time

The average experimental $k_H$ values from this study and corresponding $\gamma_i^\infty$s are summarized in Table 6.4 along with $\phi_i^{sat}$ and $\Psi$ values used in the calculations when the solute is a liquid or solid, respectively. The number of experiments at each temperature, $N$, and the standard deviation of the $k_H$ average, $s_{kH}$, are included. Also given are the average $k_H$ 95% confidence intervals (CIs) calculated using a Student's T distribution. The CIs are reported as a percentage of the average. For some compounds, $B_{ii}$ values were unavailable from the DIPPR®801 [117] database at the experimental temperatures, so in these cases $\phi_i^{sat}$ was assumed to be unity. The $\phi_i^{sat}$ values for 1,2-difluorobenzene indicate that this assumption was valid since the values are close to unity. The reported $\gamma_i^\infty$ standard deviations, $s_{\gamma\infty}$, were determined using the $s_{kH}$ values and propagation of error. For compounds where $\phi_i^{sat}$ was assumed to be unity, the $\phi_i^{sat}$ error was assumed to be 10% in the propagation of error calculations. This is a conservative error estimation since the 1,2-difluorobenzene values indicate a difference of 1-2% from unity. In some instances the errors associated with $\gamma_i^\infty$ are significantly larger than those associated with $k_H$ due to the uncertainty of $\phi_i^{sat}$ or $\Psi$. Details about each experimental run are included in Appendix D.

Figure 6.3 shows the 1,2,3-trichlorobenzene $k_H$ values obtained in this study along with those found in the literature. There are many literature values for 1,2,3-trichlorobenzene and considerable scatter in the literature values. There are also inconsistent temperature trends among the extant data. The measurements made in this study provide a strong linear trend with small uncertainty in the temperature dependence. The temperature trend of this study is in good agreement with the data of reference h [205]. While the temperature-dependent slope of the values reported by reference c [206] is consistent with the results obtained here, their absolute values appear too high at any given temperature. Much of the other literature data are scattered about the values reported here but do not provide a clear temperature-dependent trend owing to the magnitude of that scatter.

Table 6.4: $k_H$ and $\gamma_i^\infty$ values at ambient pressure (approximately 12.5 psia) from this study and literature

| T/K | $k_H$/kPa | $s_{kH}$/% | N | CI/% $\alpha = 0.05$ | Lit. $k_H$/kPa | $\phi_i^{sat}$ | $\Psi$ | $\gamma_i^\infty$ | $s_{\gamma\infty}$/% |
|---|---|---|---|---|---|---|---|---|---|
| Anisole | | | | | | | | | |
| 280.95 | $8.35\cdot10^2$ | 10 | 5 | 12 | | 1[a] | - | $5.60\cdot10^3$ | 14 |
| 293.16 | $1.48\cdot10^3$ | 4.4 | 6 | 4.6 | $1.48\cdot10^3$[206][b] | 1[a] | - | $4.23\cdot10^3$ | 11 |
| 308.15 | $2.95\cdot10^3$ | 5.6 | 4 | 8.8 | | 1[a] | - | $3.32\cdot10^3$ | 12 |
| 322.90 | $5.72\cdot10^3$ | 3.6 | 5 | 4.5 | | 1[a] | - | $2.83\cdot10^3$ | 11 |
| 1,2-Difluorobenzene | | | | | | | | | |
| 298.19 | $4.35\cdot10^4$ | 2.3 | 4 | 3.6 | $3.95\cdot10^4$ [207][c] | 0.991 | - | $6.13\cdot10^3$ | 10 |
| 308.12 | $6.65\cdot10^4$ | 3.6 | 3 | 9.0 | | 0.988 | - | $5.89\cdot10^3$ | 11 |
| 317.90 | $9.33\cdot10^4$ | 2.7 | 3 | 6.7 | | 0.984 | - | $5.41\cdot10^3$ | 10 |
| 322.89 | $1.05\cdot10^5$ | 6.4 | 5 | 7.9 | | 0.982 | - | $4.94\cdot10^3$ | 12 |
| 4-Bromotoluene | | | | | | | | | |
| 293.10 | $1.18\cdot10^4$ | 1.6 | 3 | 4.0 | | - | 0.870 | $9.04\cdot10^4$ | 26 |
| 298.16 | $1.71\cdot10^4$ | 6.0 | 3 | 15 | $1.77\cdot10^4$[208][c] | - | 0.965 | $9.41\cdot10^4$ | 26 |
| 308.10 | $2.76\cdot10^4$ | 5.1 | 12 | 3.2 | | 1[a] | - | $8.30\cdot10^4$ | 12 |
| 318.03 | $4.03\cdot10^4$ | 11 | 2 | 95 | | 1[a] | - | $6.92\cdot10^4$ | 15 |
| 322.91 | $5.28\cdot10^4$ | 2.3 | 3 | 5.7 | | 1[a] | - | $6.99\cdot10^4$ | 11 |
| 1,2,3-Trichlorobenzene | | | | | | | | | |
| 280.95 | $3.36\cdot10^3$ | 8.9 | 3 | 22 | $3.01\cdot10^3$[205][b,d] | - | 0.440 | $4.34\cdot10^5$ | 17 |
| 293.06 | $6.84\cdot10^3$ | 5.0 | 4 | 7.9 | | - | 0.535 | $3.27\cdot10^5$ | 11 |
| 308.14 | $1.44\cdot10^4$ | 6.4 | 5 | 7.9 | | - | 0.703 | $2.34\cdot10^5$ | 8.8 |
| 322.99 | $2.81\cdot10^4$ | 12 | 8 | 10 | | - | 0.946 | $1.83\cdot10^5$ | 13 |
| 2,4-Dichlorotoluene | | | | | | | | | |
| 280.94 | $7.14\cdot10^3$ | 21 | 4 | 33 | | 1[a] | - | $4.39\cdot10^5$ | 23 |
| 293.09 | $1.68\cdot10^4$ | 15 | 14 | 8.6 | | 1[a] | - | $3.99\cdot10^5$ | 18 |
| 308.15 | $3.25\cdot10^4$ | 24 | 5 | 30 | $3.38\cdot10^4$[8][c] | 1[a] | - | $2.66\cdot10^5$ | 27 |
| 323.10 | $7.54\cdot10^4$ | 20 | 4 | 32 | | 1[a] | - | $2.41\cdot10^5$ | 23 |

[a] $\phi_i^{sat}$ error of 10% assumed for propagation of error

[b] 291.15 K

[c] from $P_i^{sat}/x_i^{aq}$ at 298.15 K

[d] 277.15 K

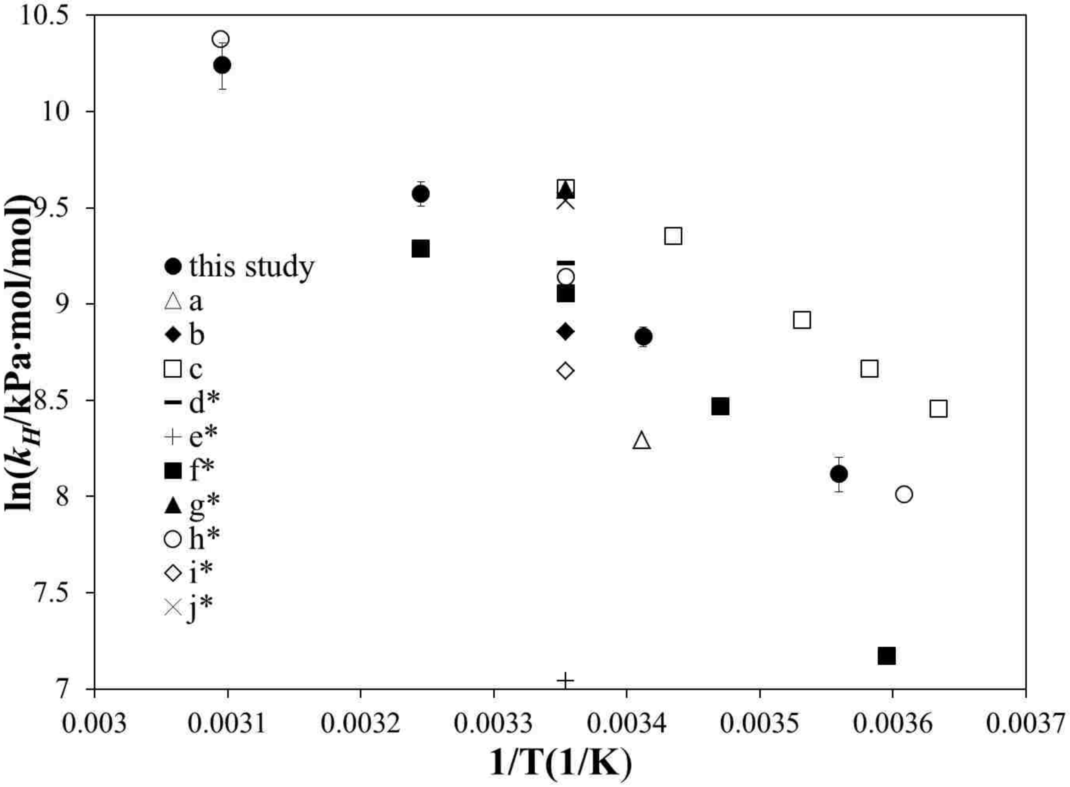

Figure 6.3: 1,2,3-Trichlorobenzene $k_H$ values from this study and from literature. Values from references marked with an asterisk (*) are $x_i^{aq}$ data converted to $k_H$ values using Equation 4.1. References: a [209], b [71], c [206], d* [210], e* [211], f* [212], g* [213], h* [205], i* [207] , j* [214]

Figure 6.4 shows the anisole $k_H$ values obtained in this study along with those found in the literature. The measurements from this study show good agreement with the anisole $x_i^{aq}$ data at higher temperatures and match the directly reported $k_H$ values at the lower temperatures. The $k_H$ values obtained from the literature $x_i^{aq}$ data are considered to be low in the lower temperature range. This means that the literature anisole $x_i^{aq}$ values at the lower temperatures have higher errors than the rest of the $x_i^{aq}$ data set.

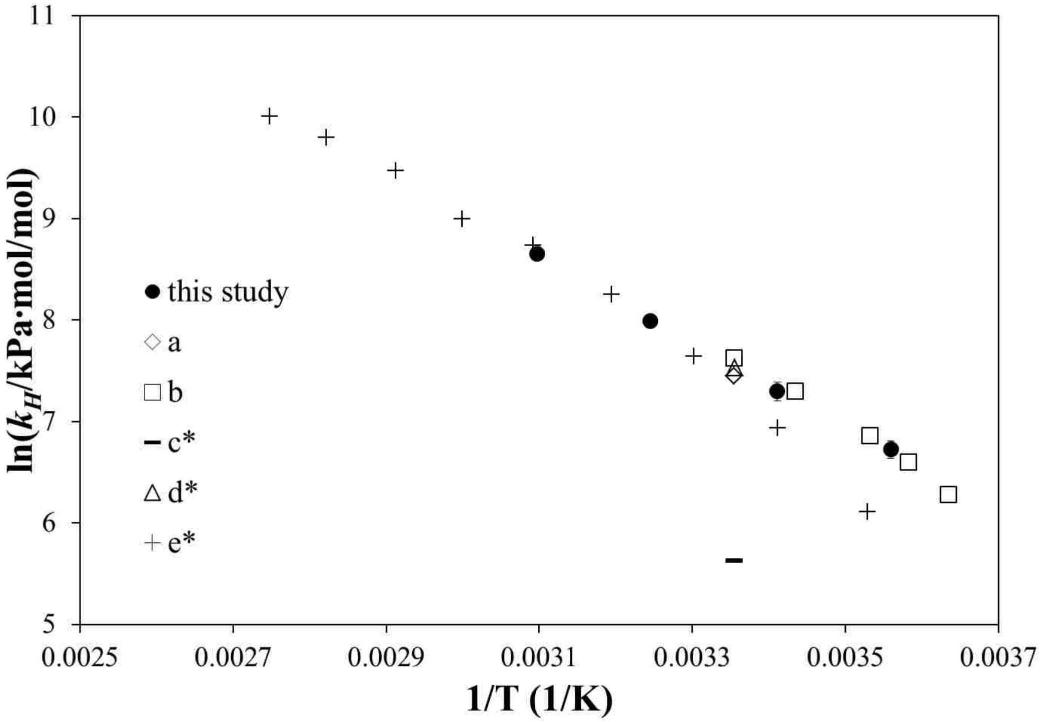

Figure 6.4: Anisole $k_H$ values from this study and from the literature. Values from references marked with an asterisk (*) are $x_i^{aq}$ data converted to $k_H$ values using Equation 4.1. References: a [172], b [206], c* [215], d* [118], e* [216]

The 2,4-dichlorotoluene results are shown in Figure 6.5. The results from this study fall within the trend of the literature $x_i^{aq}$ data. The remaining compounds have very little literature data available for comparison. Figure 6.6 shows the 1,2-difluorobenzene results from this study with the single literature $x_i^{aq}$ value. The difference between the literature value and the value from this study at the same temperature could reasonably be due to experimental uncertainty. The 4-bromotoluene results are shown in Figure 6.7. The data of this study agree the best with the literature $x_i^{aq}$ value.

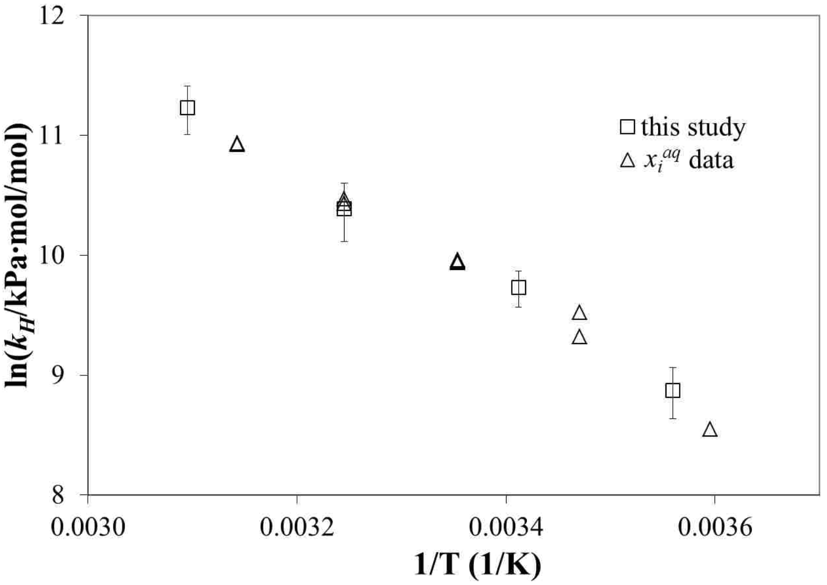

Figure 6.5: 2,4-Dichlorotoluene $k_H$ values from this study and from the literature. Values from $x_i^{aq}$ data were converted to $k_H$ values using Equation 4.1. Reference: [8]

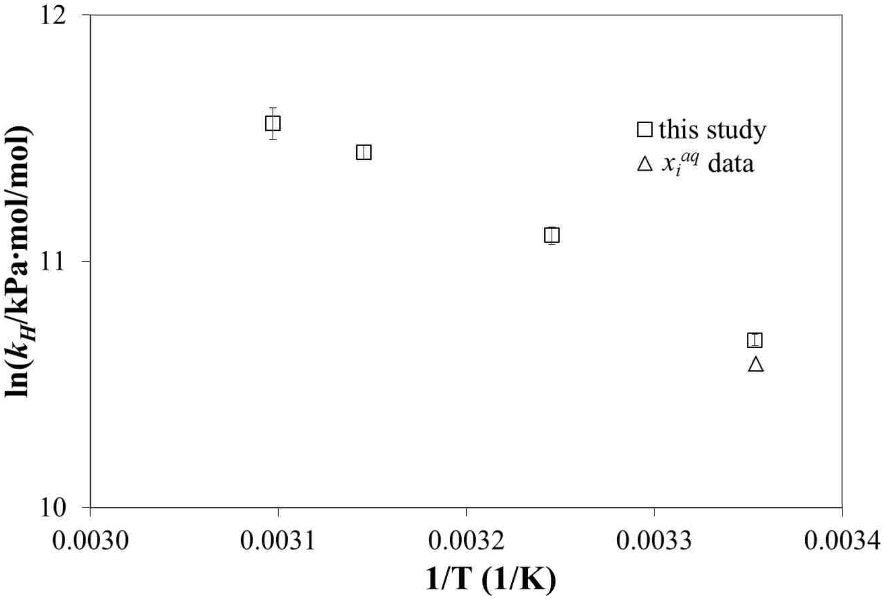

Figure 6.6: 1,2-Difluorobenzene $k_H$ values from this study and from the literature. Values from $x_i^{aq}$ data were converted to $k_H$ values using Equation 4.1. Reference: [207]

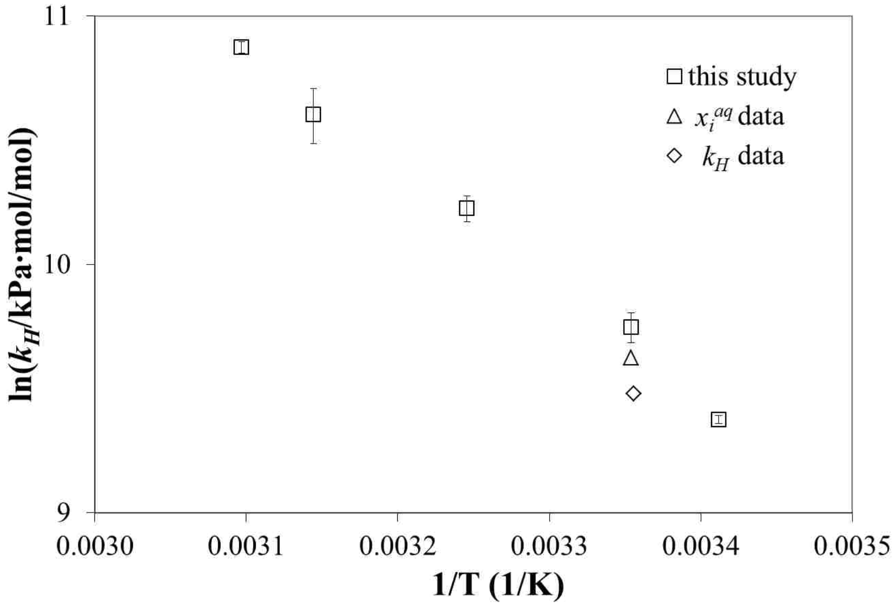

Figure 6.7: 4-Bromotoluene $k_H$ values from this study and from the literature. Values from $x_i^{aq}$ data were converted to $k_H$ values using Equation 4.1. References: [47, 208]

The experimental results from this study clarify discrepancies between literature values for 1,2,3-trichlorobenzene and anisole. Temperature-dependent values were determined for 2,4-dichlorotoluene, 1,2-difluorobenzene, and 4-bromotoluene which only had limited literature data. Properties in the DIPPR®801 database allowed for the determination of $\gamma_i^\infty$ values for each compound. A fugacity ratio was required to determine $\gamma_i^\infty$ values for the solid solutes. In addition, a procedure was identified for determining when adsorption effects become significant during IGS experiments.

# 7 Prediction Methods

## 7.1 Overview of Prediction Method Types

This section provides general information about the types of prediction methods available in the literature. Property-property relationships (PPRs) relate the property of interest to other properties of the chemical [24]. These relationships can be thermodynamically based or strictly empirical. PPRs are often restricted to the chemical classes from which they were derived [217].

Group-contribution methods (GCMs) parse the chemical's structural formula into functional groups and fragments, and the property of a compound is estimated by summing together the contributions of each segment [218]. First-order methods use groups that do not take into account interactions with neighboring compounds. Second-order methods are more complex because neighboring atoms are included in the group definitions. Limitations of these methods are their inability to differentiate between isomers and large errors for compounds with multiple non-alkyl functional groups. Empirical corrections are often used to offset these deviations. Group-contribution methods fail when a compound contains a functional group that was not contained in the original training set of the method [14, 219]. Bond contribution methods (BCMs) work in a similar fashion; they add up the contributions from each bond in the molecule.

Quantitative structure-property relationships (QSPRs) are based on fragment contributions and structural descriptors [24]. Descriptors (such as topological indices, molecular volume, molecular surface area, etc.) are calculated from molecular structure [220]. There are various software tools and methods for obtaining and selecting descriptors with some being more complex than others. Another name associated with methods of this type is quantitative structure-activity relationships (QSARs).

Linear Solvation Energy Relationships (LSERs) relate the Gibbs energy of solution of a solute to a series of empirical parameters that describe the cavity formation and the solute-solvent interaction processes that occur when a gaseous solute dissolves in a liquid [221]. LSERs are a type of QSPR [222]. Parameters used (often called “solvatochromic parameters”) include solute dipolarity/polarizability, hydrogen bond donor acidity, and hydrogen bond acceptor basicity. These parameters originate from experimental data which are not always available for every compound.

Molecular simulations (such as Monte Carlo) and quantum mechanical methods (such as continuum-solvation models) have high computational costs making them difficult to use for predicting properties of large groups of compounds [219, 223]. A continuum-solvation model (CSM) that has become more prominent is the Conductor-like Screening Model for Real Solvents (COSMO-RS). COSMO-RS is a surface interaction model that uses molecular charge densities obtained by molecular quantum chemical calculations [224, 225]. An advantage of COSMO-RS is that only a few adjustable parameters are required [226].

Neural networks (NN) have become more popular in prediction method development. Neural networks consist of many processing units arranged in a network [227]. The networks have an input layer, an output layer, and intermediate hidden layers. Each network unit is influenced by connected units, and the extent of influence can be changed by adjusting the weights of the connections. Learning algorithms are used to modify the system behavior by changing the values of these weights. While these methods have been shown to perform well, they are impossible to duplicate from literature articles. The model would have to be obtained from the author in order to use the method.

## 7.2 Prediction Method Selection

Most $k_H$ prediction methods only predict values at 298.15 K. Table 7.1 lists some of the available prediction methods for $k_H$ at 298.15 K. UNIFAC expansions were excluded from the table due to the large number of authors that have added to this method. Dearden and Schüürmann [14] compared 12 of these methods and found that the EPA's HENRYWIN bond contribution method [83] outperformed the other methods. Values predicted from this method have been included as constant value entries in the database. The actual method was not programmed into DIADEM because it uses hundreds of bond contributions. The software is available without cost from the EPA website. The predicted values were imported into the database from the software.

There are significantly fewer $k_H$ methods that predict temperature dependence, and it was determined that the greatest contribution can be made to these methods. An initial review was conducted on temperature-dependent prediction methods to determine the methods to include in this study. Temperature-dependent prediction methods that were excluded are listed in Table 7.2 with a brief reason for exclusion. The method of Yezdimer, Sedlbauer, and Wood (2000) [276] applies to some chemical families that were not included in the database analysis. Of the groups that applied to compounds included in this study, a similar method was published a few years later with superior contributions (see Section 7.2.1). The methods of Goss [277] and Abraham et al. [278] both require molecular descriptors that are based on experimental data. These methods were excluded due to the time that would be required to find reported descriptor values in the literature for the compounds in the database. The method of Hilal et al. [279, 280] uses two independent models to predict $x_i^{aq}$ and $P_i^{sat}$ and then calculates $k_H$ using Equation 4.1. There are publications concerning the method performance, but no publications have been found on the actual method parameters preventing the inclusion of this method in this study.

Table 7.1: $k_H$ prediction methods at 298.15 K

| Authors | Method Type | Authors | Method Type | Authors | Method Type |
|---|---|---|---|---|---|
| Hine and Mookerjee (1975) [23, 228] | (1) BCM<br>(2) GCM | Cramer and Truhlar (1992) [262] | CSM | Dearden et al. (2000) [249] | QSPR |
| Cramer (1980) [230] | QSPR | Jorgensen and Nguyen [263] (1993) | Monte Carlo | Meylan and Howard (2000) [219] | (1) BC &<br>(2) GC |
| Cabani (1981) [232] | GCM | Myrdal (1994) [265] | PPR | Öberg (2001) [252] | QSPR |
| Shiu and Mackay (1986) [234] | PPR | Abraham et al. (1994) [267] | LSER | Ferreira (2001) [254] | QSPR |
| Jin et al. (1986) [236] | GCM | Schüürmann (1995) [269] | CSM | Yao et al. (2002) [256] | QSPR |
| Nirmalakhandan and Speece (1988) [238] | QSPR | Chambers et al. (1996) [271] | CSM | Lin and Sandler (2002) [218] | GCM |
| Hawker (1989) [23, 240] | QSPR | Dearden et al. (1997) [272] | QSPR | Yaffe et al. (2003) [259] | QSPR with NN |
| Sabljic and Gusten (1989) [23, 242] | QSPR | Schüürmann (1997) [274] | software | Modarresi et al. (2005) [261] | QSPR |
| Brunner et al. (1990) [23, 248] | QSPR | Barone et al. (1997) [229] | CSM | Modarresi et al. (2007) [219] | QSPR |
| Crovetto et al. (1990) [250] | PPR | Hawkins et al. (1997) [231] | CSM | Schröder et al. (2010)[264] | COSMO-RS |
| Meylan and Howard (1991) [251] | BCM | Hawkins et al. (1998) [233] | CSM | Gharagheizi et al. (2010) [266] | GCM with NN |
| Yaws et al. (1991) [13], (2010) [253] | Must be bought | Katritzky et al. (1998) [235] | QSPR | Goodarzi et al. [268] | QSPR with NN |
| Suzuki et al. (1992) [255] | GCM & QSPR | Famini et al. (1999) 32 [237] | LSER | Peterson (2011) [270] | QSPR |
| Russell et al. (1992) [257] | QSPR | Cash (1999) [239] | QSPR | Gharagheizi et al. (2010) [266] | GCM with NN |
| Dunnivant et al. (1992) [258] | QSPR | Gramatica et al. (1999) [241] | QSPR with NN | Raventos-Duran (2010) [273] | GCM |
| Cramer and Truhlar 36 [260](1992) | CSM | Plyasunov and Shock (2000) [243] (2004) [244] (2005) [245] (2006) [246, 247] | GCM | Sahoo (2011) [275] | QSPR |

Table 7.2: $k_H$ temperature-dependent prediction methods excluded from this study

| Author | Method Description | Reason for Exclusion |
|---|---|---|
| Yezdimer, Sedlbauer, and Wood (2000) [276] | GCM; need water equation of state | Similar, superior method published later |
| Goss (2006) [277] | LSER | Difficulty in obtaining descriptors |
| Abraham et al. (2007) [278] | LSER | Difficulty in obtaining descriptors |
| Nirmalakhandan et al. (1997) [281] | QSPR | Does not apply to very many compounds |
| Huang et al. (2009) [282] | Molecular Simulation | Computational cost and difficulty obtaining models |
| Hilal et al. (2008) [279, 280] | SPARC-solvation model | Publications on method performance but not method parameters |

Table 7.3 lists the temperature-dependent prediction methods that have been programmed into DIADEM along with the type of method and the applicable compounds. The GCM and BCM methods developed by Lau et al. [39] are applicable for different chemical families. The chemical families that do not overlap between the methods are italicized. Initially the plan was to add to one of these existing methods. However, it was decided to develop a completely different method. The methods listed in Table 7.3 are described in more detail along with reasons they were not expanded in this study. A quantitative comparison of the methods is provided in Section 7.2.5.

Table 7.3: $k_H$ temperature-dependent prediction methods chosen for evaluation

| Author | Method Description | Applicable compounds | |
|---|---|---|---|
| Sedlbauer et al. (2002) [191], (2007) [283] and (2008) [22] | GCM; need water equation of state | alkanes, alkenes, alkyl phenols, alkyl anilines, aromatic hydrocarbons, cycloalkanes, $H_2S$, and $CO_2$ | |
| Plyasunov and Shock (2003) [284] | GCM | substructural parameters with atom types C, H, N, O, F, Cl, Br, I, and S | |
| Kühne, Ebert, and Schüürmann (2005) [285] | GCM & BCM; need a reference value | substructural parameters with atom types C, H, N, O, F, Cl, Br, I, and S | |
| Lau, Rogers, and Zei (2010) [39] | Separate GCM & BCM; need a reference value | GCM: alkanes, cycloalkanes, *cycloalkenes*, alkylbenzenes, *primary alcohols*, *secondary alcohols*, aliphatic chlorides, ketones | BCM: alkanes, *alkenes*, cycloalkanes, alkylbenzenes, aliphatic chlorides, ketones |

### 7.2.1 Method of Sedlbauer et al. [22, 191, 283]

This method was initially published for aqueous hydrocarbons by Sedlbauer, Bergin, and Majer in 2002 [191]. In 2008, the same authors published additional parameters for $CH_4$, $CO_2$ and $H_2S$ [22]. Parameters for alkylphenols and alkylanilines were developed in 2007 by Čenský, Sedlbauer, Majer, and Růžička [283] using the hydrocarbon parameters developed in 2002. Because these parameters can all be used together, they have been lumped together as one method even though the parameters were published in three separate papers.

In addition to predicting $k_H$, this method also predicts models for derivative properties (Equations 2.4-2.7). Experimental data related to the derivative properties were used in addition to $k_H$, $x_i^{aq}$, and $\gamma_i^{\infty}$ data to develop this prediction method. The experimental data were simultaneously fit to a semitheoretical hydration model that uses the derivative property relationships. Group contribution values are used to calculate a reference value at $T_{ref}$ and $P_{ref}$ (298.15 K and 0.1 MPa), and a separate set of group contribution values are used to model the temperature and pressure dependency. The Plyasunov and Shock [243] group contribution values at reference conditions were used for hydrocarbons. The hydration model requires properties of water that can be calculated using an equation of state. Sedlbauer et al. [22, 191, 283] used the equation of state by Hill [286]. The IAPWS-95 [287] equation of state was used when programming this method into DIADEM. This difference should not affect method performance.

This method applies to hydrocarbons up to temperatures and pressures of approximately 570 K and 100 MPa, respectively. This broad range allows the prediction method to be applicable for systems encountered in the oil and natural gas industries. Since this method is both a function of temperature and pressure and DIADEM allows for one dependent variable, the variable of pressure was “removed” by using the DIPPR® 801 liquid density equation for water (which only has the dependent variable of temperature) in all calculations that required density. This results in thermodynamic properties of water along the saturation line.

This method was not chosen for expansion in this study because derivative properties were not included in the database. In addition, this model extends beyond the temperature and pressure scope of the data evaluated in this study.

### 7.2.2 Method of Plyasunov and Shock [284]

The method of Plyasunov and Shock [284] is a group contribution method that predicts values of the vapor-liquid distribution coefficient ($K_D$) from 273 K to the critical temperature of water (647.1 K). $K_D$, is related to $k_H$ by:

$$k_H = K_D \phi_i^\infty P_{solv}^{sat},$$

where $\phi_i^\infty$ is the fugacity coefficient of the solute at infinite dilution and $P_{solv}^{sat}$ is the vapor pressure of water. The method includes group contribution values of $\phi_i^\infty$ allowing for $k_H$ to be calculated. High-temperature calculations are based on the Krichevskii parameter. This method uses water vapor pressure, and liquid and vapor water densities obtained from the IAPWS-95 equation of state [287]. This model was developed for hydrothermal geochemical applications which are interested in high-temperature and high-pressure values.

The Plyasunov and Shock method [284] was not the most accurate of the prediction methods evaluated in this study which is possibly due to the target temperature range of applicability. This method may be more accurate at near-critical conditions compared to methods that were developed using data closer to ambient conditions. However, the prediction capabilities of this method at high temperatures and pressures were not determined because these conditions are beyond the scope of the data evaluated in this study. This method was not chosen for additional development or refinement due to the temperature scope of data included in this project. In addition, any development of this method would require Krichevskii parameters which were not included in the database.

### 7.2.3 Methods of Lau et al. [39]

Lau et al. [39] published separate bond and group contribution methods in the same paper. From a statistical standpoint, these methods are equivalent in their prediction capabilities. There are differences in the chemical families covered by both methods as indicated in Table 7.3. The chemical families that do not overlap between the methods are italicized. Temperature dependence is modeled using a variation of DIPPR® 801 Equation 101 (see Table 4.3),

$$\ln\left(\frac{k_H}{k_{H,ref}}\right)=\left(\sum_i B_i n_i\right)\left(\frac{1}{T_{ref}}-\frac{1}{T}\right)+\left(\sum_i C_i n_i\right)\left(\ln\left(\frac{T}{T_{ref}}\right)\right), \qquad 7.1$$

where $B_i$ and $C_i$ are group contribution values for fragment $i$, $n_i$ is the number of times a group occurs, $T$ is temperature, and superscript *ref* refers to a reference value obtained from experimental data or a prediction method. Since $\ln(k_H)$ is related to $\Delta G_{hyd}^{\infty}$ (Equation 2.4), coefficients "*B*" and "*C*" are related to $\Delta H_{hyd}^{\infty}$ (through integration of Equation 2.5) and $\Delta Cp_{hyd}^{\infty}$ (through integration of Equation 2.6), respectively. Both the bond and group contribution methods predict coefficients "*B*" and "*C*" given in Equation 7.1. This method was not chosen for expansion in this study due to the requirement of a reference value. In addition, some of the group (and/or bond) contributions were developed on limited data. More data for similar compounds are available in the 801E database.

### 7.2.4 Method of Kühne, Ebert, and Schüürmann [285]

The method of Kühne et al. [285] predicts temperature-dependence using an abbreviated form of Equation 7.1. This method uses group contribution values and correction factors to predict coefficient "*B*", so it only predicts a linear relationship between $\ln(k_H)$ and inverse temperature. Therefore, it can only be applied over a more limited range of temperature than the method of Lau et al. [39]. Out of the temperature-dependent methods programmed into DIADEM, this method has the widest chemical family applicability. This method was not chosen for expansion due to its limited temperature applicability and the requirement of a reference value.

### 7.2.5 Existing Method Comparison

The prediction methods were compared using data for 157 compounds. Some of the methods apply to compounds outside of the chemical families included in the comparison. Only the compounds included in later method development were included to make the comparisons more meaningful. The number of applicable compounds (nC) and the average absolute deviations (AAD) for each chemical family and method are summarized in Table 7.4. Also included is a breakdown of the AAD based on the error of the experimental data.

The methods of Plyasunov and Shock [284] and Kühne et al. [285] apply to all of the compounds included in the comparison, but the method of Kühne et al. [285] has a smaller overall AAD. The Lau et al. [39] methods have comparable overall performances, but the group-contribution method applies to more of the compounds included in the comparison. The Lau et al. [39] methods are better than the Kühne et al. [285] method, and this can be attributed to the additional temperature-dependent coefficient. The Sedlbauer et al. [22, 191, 283] method applies to the smallest group of compounds. It does not perform as well as the Lau et al. [39] methods. However, the Lau et al. [39] methods use an experimental reference value whereas the Sedlbauer et al. [22, 191, 283] method is completely predictive.

## 7.3 Prediction Method Development

While the Kühne et al. [285] and Lau et al. [39] methods have reasonable prediction capabilities, they both require a reference value. The reference value can be an experimental value or it can predicted using a separate prediction method. Prediction methods that can be used to calculate a reference value are not available that use the same group definitions as Kühne et al. [285] or Lau et al. [39]. It was decided that a prediction method would be developed that uses the same group definitions for all parameters including the reference value. This simplifies the calculations because each compound only has to be parsed once.

Initially efforts were made to develop a group contribution method that predicted coefficients "*A*", "*B*", and "*C*" of DIPPR® Equation 101 simultaneously. This did not work well due to the high number of parameters. Instead, it was decided to use the method of Plyasunov et al. [243] for the reference values, and then develop a model using the same group definitions to predict coefficients "*B*" and "*C*" in Equation 7.1. Sedlbauer et al. [191] uses the method of Plyasunov et al. [243] as a reference point in their prediction method. Plyasunov et al. [243] did a thorough literature review of $k_H$ and derivative property data for hydrocarbons. They provided recommended values for each compound and developed their prediction methods based on these values. While this method is more limited in chemical applicability than the HENRYWIN bond-contribution method [83], the method is more reliable due to the data used for method development.

Table 7.4 Temperature-dependent $k_H$ prediction method comparison for select compounds

| Method | Plyasunov and Shock AAD% | nC | Kühne | nC | Lau GCM AAD% | nC | Lau BCM AAD% | Comps | Sedlbauer AAD% | nC |
|---|---|---|---|---|---|---|---|---|---|---|
| Overall | 139.8 | 157 | 40.4 | 157 | 16.9 | 98 | 13.8 | 69 | 30.1 | 46 |
| Acetates | 71.8 | 14 | 15.2 | 14 | - | - | - | - | - | - |
| Aliphatic ethers | 176.8 | 11 | 18.6 | 11 | - | - | - | - | - | - |
| Dimethylalkanes | 87.4 | 6 | 113.8 | 6 | 12.7 | 6 | 12.6 | 6 | 65.7 | 6 |
| Formates | 84.3 | 7 | 14.9 | 7 | - | - | - | - | - | - |
| Ketones | 91.9 | 24 | 34.6 | 24 | 39.5 | 21 | 23.6 | 22 | - | - |
| Methylalkanes | 43.9 | 8 | 18.3 | 8 | 3.9 | 8 | 4.0 | 8 | 20.8 | 8 |
| *n*-alcohols | 62.9 | 10 | 29.7 | 10 | 14.5 | 10 | - | - | - | - |
| *n* -alkanes | 64.3 | 14 | 102.6 | 14 | 11.9 | 14 | 12.2 | 14 | 32.1 | 14 |
| *n* -alkylbenzenes | 139.2 | 8 | 18.5 | 8 | 7.8 | 8 | 7.7 | 8 | 19.0 | 8 |
| Other aliphatic alcohols | 87.9 | 21 | 20.5 | 21 | 11.5 | 21 | - | - | - | - |
| Other alkanes | 82.0 | 2 | 14.8 | 2 | 11.2 | 2 | 2.7 | 2 | 24.2 | 2 |
| Other alkylbenzenes | 949.3 | 9 | 145.0 | 9 | 10.5 | 8 | 10.1 | 9 | 22.0 | 8 |
| Other ethers/diethers | 92.3 | 5 | 10.9 | 5 | - | - | - | - | - | - |
| Other polyfunctional C, H, O | 97.9 | 2 | 10.6 | 2 | - | - | - | - | - | - |
| Other saturated aliphatic esters | 84.0 | 3 | 31.0 | 3 | - | - | - | - | - | - |
| Propionates and butyrates | 93.6 | 13 | 26.4 | 13 | - | - | - | - | - | - |
| < 1% | 81.1 | 1 | 11.6 | 1 | 2.1 | 1 | 4.7 | 1 | 24.2 | 1 |
| < 3% | 74.2 | 11 | 11.9 | 11 | 4.5 | 8 | 4.3 | 7 | 11.3 | 7 |
| < 5% | 112.3 | 27 | 23.8 | 27 | 6.3 | 19 | 6.0 | 12 | 14.9 | 9 |
| < 10% | 119.0 | 77 | 36.2 | 77 | 10.4 | 52 | 8.4 | 34 | 21.1 | 19 |
| < 25% | 124.0 | 71 | 51.8 | 71 | 33.7 | 43 | 28.5 | 28 | 41.0 | 16 |
| < 50% | 161.8 | 34 | 49.7 | 34 | 36.5 | 27 | 35.0 | 19 | 48.1 | 15 |
| < 100% | 513.8 | 15 | 65.3 | 15 | 76.2 | 9 | 75.4 | 8 | 77.5 | 6 |

Initially Plyasunov et al. [243] developed a first-order group contribution prediction method for hydrocarbons and alcohols. Additional functional group contribution terms were added to their method in later publications [245-247, 288]. In these later publications, second-order group contribution parameters were also developed. However, second-order hydrocarbon groups were not defined for all of the hydrocarbons included in the original first-order method. In this study, both the first- and second-order methods were expanded.

The method of Plyasunov et al. [243] uses the relationship between $k_H$ and $\Delta G_{hyd}^{\infty}$ (Equation 2.4). Plyasunov et al. [243] define the standard state in terms of molality (standard molality of 1 mol/1000 g at a $P_{ref}$ of 100 kPa), so a unit conversion must be used with the definition of $k_H$ in this study,

$$RT\ln\left(\frac{k_H}{P_{ref}\cdot N_W}\right)=\Delta G_{hyd}^{\infty}, \qquad 7.2$$

where $N_W$ = (1000 g/1 mol)/(18.0153 g/mol) ≈ 55.5084 (mol/mol). The group contribution values determined by Plyasunov et al. [243] are given in terms of $\Delta G_{hyd}^{\infty}$. For the first- and second-order methods of this study, values for $k_{H,ref}$ are calculated using Equation 7.2. Using a group contribution scheme, any property ($Y$) can be determined by:

$$Y=Y^0+\sum_i n_iY_i \qquad 7.3$$

where $n_i$ is the number of a times group $i$ appears in the compound, $Y_i$ is the contribution of the group to the overall property, and $Y^0$ is a constant. Plyasunov and Shock [243] defined a $Y^0$ value of 7.95 kJ/mol for $\Delta G_{hyd}^{\infty}$ based on theoretical models (the contribution of a material point). The $Y^0$ values for $B$ and $C$ are 0 for the first- and second-order methods of this study.

### 7.3.1 Data Selection

The first step was selecting the data to use in method development. The recommended values at 298.15 K of this study were used in constant value (or reference value) method development. With temperature-dependent models, there are multiple ways that data are used.

1. Regression coefficients are determined from the data, and the prediction method is then developed from the regression coefficients (*A*, *B*, *C*, etc.) and not directly from data. Examples are the methods of Kühne et al. [285], Nagvekar [289], Hsu [290].
2. Regression coefficients are determined from the data, and values are calculated at equal temperature intervals (such as every 10 K) using the regression. The prediction method is developed from these values. Examples include prediction methods developed by Elbro et al. [291] and Harrison [292].
3. Prediction method is developed directly from data.

The first two options were not used due to the different temperature ranges of available data. The coefficients obtained in the data analysis of this study do not refer to the same temperature ranges. In addition, a second temperature-dependent coefficient is not statistically significant for some compounds due to the limited data. A combination of Options 2 and 3 was determined to be the best method. The data were not used directly due to the extreme distribution of the number of points per compound in addition to the experimental error. For example, benzene has 341 experimental points whereas 1,2,3,4-tetramethylbenzene has 3 experimental points. Smoothed values were calculated from the regressions obtained in the data analysis process at every unique temperature found within the data of a given compound. For example, if data are available for a compound at temperatures of 275 K, 298 K, 298 K, and 330 K, values calculated from the regression at 275 K, 298 K, and 330 K were included in the method development. The uncertainties assigned to the regression (determined from 95% confidence intervals during data analysis) were then assigned to these smoothed points. Compounds with more temperature-dependent data will also inherently have more weight due to the existence of more unique temperatures.

A similar process was used for the data of compounds in which the API regression was accepted (see Section 4.5). The unique temperatures of the data in the 801E database were determined for a given compound. The Smoothed values were determined using the API regressions.

A weighted least-squares procedure was used to determine the group contribution values. The objective function, $O$, to be minimized is defined by

$$O = \sum_i \left[ \frac{\ln k_H^{\text{mod},i} - \ln k_H^{\exp,i}}{\sigma_i} \right]^2 , \qquad 7.4$$

where $\ln k_H^{mod,i}$ are the natural log values calculated from the model, $\ln k_H^{exp,i}$ are the natural log experimental values, and $\sigma_i$ is the uncertainty (on a natural log scale) of the Smoothed value. By using weighted values, Smoothed values with smaller uncertainty will be given greater weight in the regression. In this study, the weighted least-squares procedure was completed using SAS® software.

### 7.3.2 Validation Techniques

A general procedure was used multiple times throughout method development. Approximately 10% of the compounds were assigned to a validation set. The remaining compounds (training set) were then randomly divided into 10 subsets to perform a 10-fold cross-validation. In the 10-fold cross-validations, a single subset of the training set was reserved as a prediction set and the remaining 9 were used as a learning set. A preliminary model was developed using the learning set and applied to the prediction set. This process was repeated so that each subset was used as the prediction set once. The statistics from the 10 iterations were averaged to provide a better estimation of the overall method accuracy. The entire training set was then used to develop model parameters. The model was finally applied to the validation set as an additional check on the method performance.

The average absolute deviation (AAD) is given by:

$$AAD = \sum_{i=1}^{n} \frac{\left| k_H^{\mathrm{mod},i} - k_H^{\exp,i} \right|}{k_H^{\exp,i}} . \tag{7.5}$$

The AAD is calculated on a normal scale and not a log scale to provide better insight of the method performance. Also reported is the Pearson's product moment correlation coefficient, $R^2$, (the $R^2$ value returned by the Microsoft Excel® RSQ function) given by

$$R^2 = \frac{\sum_{i}^{n} (\ln k_H^{\mathrm{mod},i} - \ln k_H^{\mathrm{mod},avg})(\ln k_H^{\exp,i} - \ln k_H^{\exp,avg})}{\sqrt{\sum_{i}^{n} (\ln k_H^{\mathrm{mod},i} - \ln k_H^{\mathrm{mod},avg})^2 \sum_{i}^{n} (\ln k_H^{\exp,i} - \ln k_H^{\exp,avg})^2}} , \tag{7.6}$$

where $\ln k_H^{\exp,avg}$ is the average natural log experimental value used in the training set (or learning set during cross-validation) and $\ln k_H^{\mathrm{mod},avg}$ is the average natural log model value used in the validation set (or prediction set during cross-validation). A reliable method will have $R^2$ values that approach unity and low AADs for both the training and validation sets.

### 7.3.3 First-Order Group Contribution Method

Evaluated temperature-dependent data were available for 48 hydrocarbons. More data are available for compounds at 298.15 K; however, these compounds were not used because they would only test the validity of the Plyasunov et al. [243] method and not the temperature-dependent method. Compounds were classified as alkanes, alkenes, cycloalkane, cycloalkene, or benzene derivative, and one or two compounds were randomly chosen from each classification for the validation set. This ensured a diverse set of groups were represented in the validation set. The remaining 42 compounds (training set) were randomly divided into 10 subsets to perform a 10-fold cross-validation. The group contribution parameters were determined using the entire training set, and the prediction method was then applied to the six compounds that were initially set aside in the validation set. Results of the 10-fold cross-validation and overall method performance are summarized in Table 7.5. The statistics indicate that the method has reasonable predictive capabilities. The results are shown in Figure 7.1.

Table 7.5: Summary of performance for first-order group contribution temperature-dependent method for hydrocarbons

| Set | #Compounds | AAD | $R^2$ | 10-Fold Cross-Validation | Avg. AAD | Avg. $R^2$ |
|---|---|---|---|---|---|---|
| Training | 42 | 14% | 0.994 | Learning | 14% | 0.994 |
| | | | | Prediction | 27% | 0.951 |
| Validation | 6 | 13% | 0.993 | - | - | - |

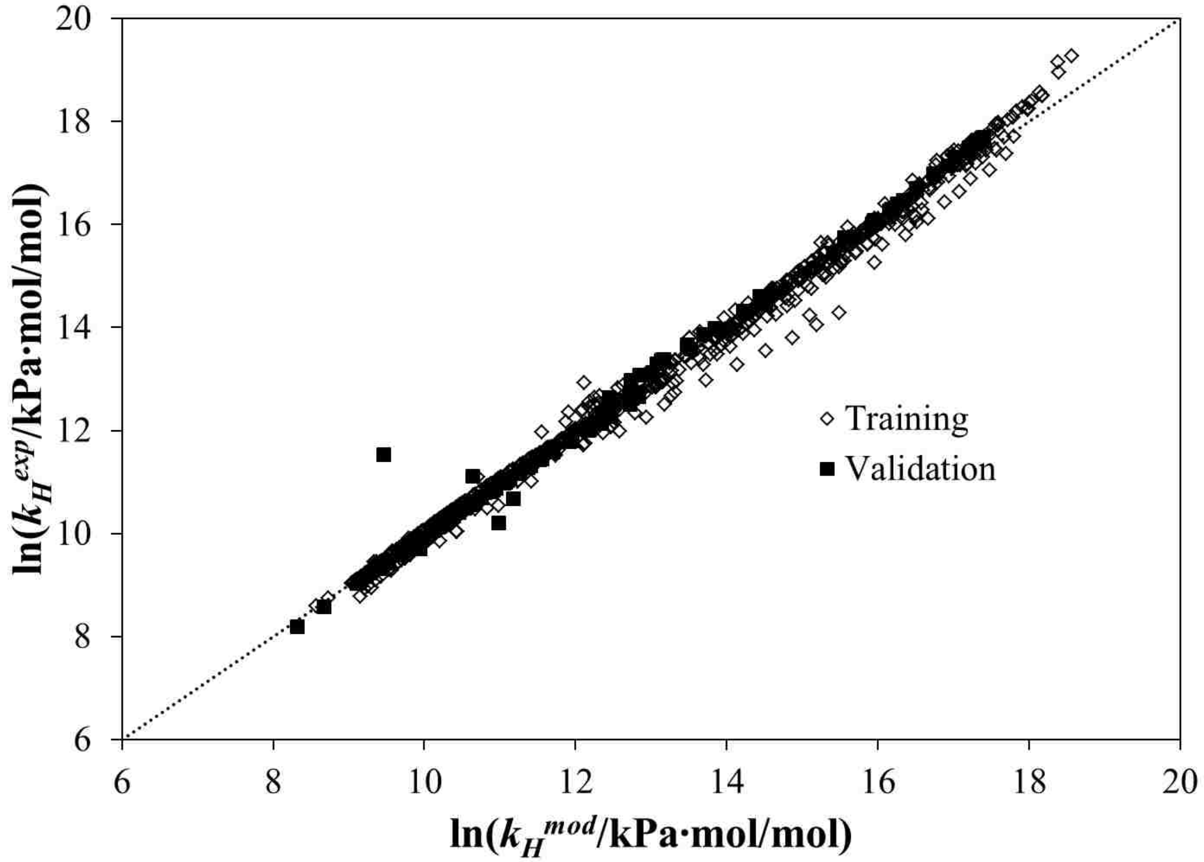

Figure 7.1: Plot of experimental versus model values for the first-order temperature-dependent group contribution method for hydrocarbons

The compound with the biggest discrepancy in the validation set is 1,4-cyclohexadiene. It is the only cycloalkene with more than one double bond. (It randomly ended up in the validation group instead of the training group.) The cyclic compounds also have the largest error in the training set. There are less data for these compounds and more uncertainty in the available data compared to the alkanes and benzene derivatives.

The method was expanded for aliphatic alcohols, ketones, and formates. Data were found for 61 compounds. Seven compounds were randomly chosen for the validation set. The remaining 54 training set compounds were divided into 10 subgroups. A 10-fold cross validation was performed as previously described. The group contribution parameters were then determined using the entire training set, and the prediction method was then applied to the seven compounds in the validation set. Results of the 10-fold cross-validation and overall method performance are summarized in Table 7.6. The results are shown in Figure 7.2.

Table 7.6: Summary of performance for first-order group contribution temperature-dependent method for alcohols, ketones, and formates

| Set | #Compounds | AAD | $R^2$ | 10-Fold Cross-Validation | Avg. AAD | Avg. $R^2$ |
|---|---|---|---|---|---|---|
| Training | 54 | 24% | 0.920 | Learning | 24% | 0.921 |
| | | | | Prediction | 29% | 0.934 |
| Validation | 7 | 33% | 0.969 | - | - | - |

The two compounds with the largest discrepancies are acetophenone and acetylacetone. Acetophenone is the only aromatic ketone included in the entire dataset, and acetylacetone is the only di-ketone included in the entire dataset. The large errors could be attributed to experimental error and/or the structures. More data from similar compounds would be necessary to determine the exact cause. The statistics given in Table 7.6 include the results of these two compounds. It is recommended that this method should only be used for alcohols, ketones, and formates that are aliphatic. In addition, correction factors might be necessary for multifunctional compounds.

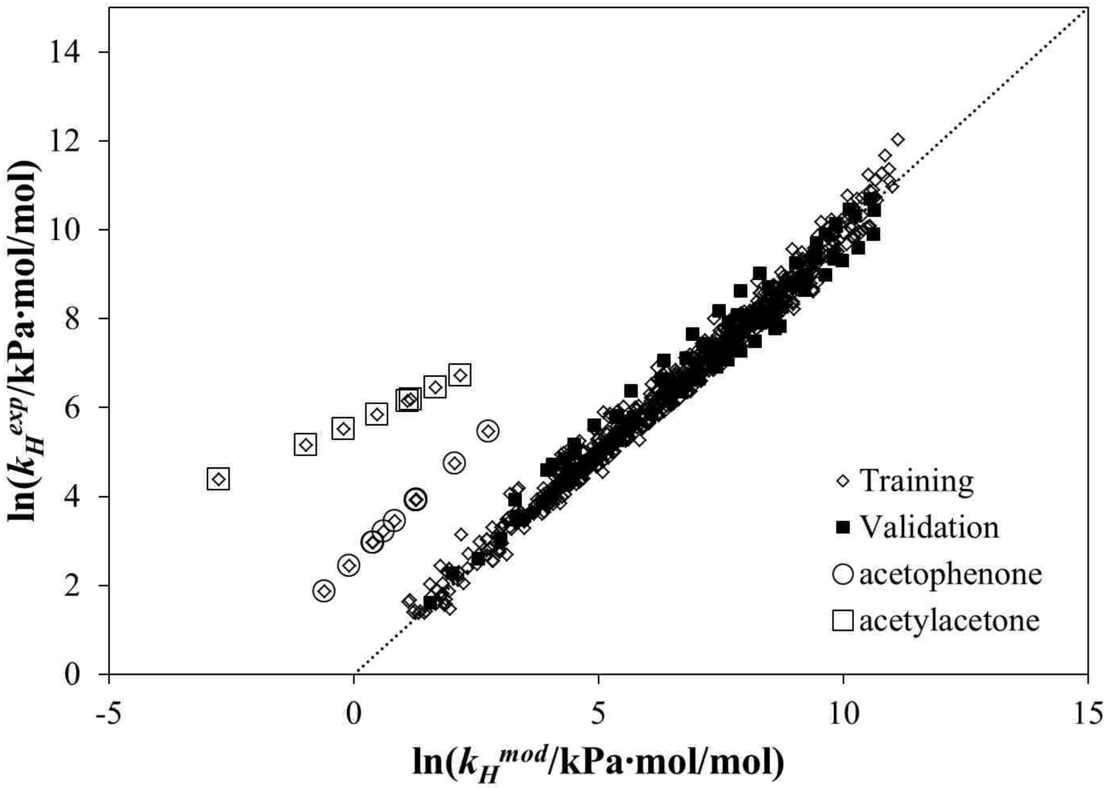

Figure 7.2: Plot of experimental versus model values for the first-order temperature-dependent group contribution method for alcohols, ketones, and formates

The temperature-dependent coefficients determined in this study are summarized in Table 7.7 along with the standard errors and two-tailed p-values. The table also includes the reference values developed by Plyasunov et al. [243-247], the number of compounds that contained a group (nC), the total number of temperature-dependent points that contained a group (nG), and the temperature range of the data used for the individual groups. Multiple coefficients have large standard errors and are not statistically significant (p-values > 0.05). In general, the groups corresponding to these coefficients do not have as much data compared to the groups with statistically significant coefficients resulting in higher uncertainty. When Plyasunov et al. initially developed the group contribution value for ketones, they did not include a correction factor [288]. A correction factor was added later for tertiary carbons attached to a ketone group [244]. The only compound influenced by this correction in the training and validation sets was diisopropyl ketone. The reference value used in method development included the correction factor. However, the correction factor was not included in the temperature-dependent development because it was not needed. Sample calculations are included in Appendix D.

Table 7.7: Summary of parameter estimates for the first-order method

| Group | $\Delta G^{\infty}_{hyd,i}$ (kJ/mol)[a] | $B_i$ | | | $C_i$ | | | Training | | Validation | | Overall Temp. Range (K) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Value (K) | SE[b] | p-value[c] | Value | SE[b] | p-value[c] | nC | nG | nC | nG | |
| c-C=C[d] | -9.47 | 94550 | 16375 | < 0.001 | -326 | 55 | < 0.001 | 3 | 24 | 1 | 12 | 273-318 |
| c-CH[d] | -1.03 | 335 | 990 | 0.74 | -3.6 | 3.0 | 0.22 | 4 | 78 | 0 | 0 | 273-444 |
| c-CH$_2$[d] | 0.83 | 3275 | 276 | < 0.001 | -8.26 | 0.82 | < 0.001 | 10 | 681 | 2 | 39 | 273-444 |
| C | -4.51 | 1203 | 2676 | 0.65 | -8.1 | 8.6 | 0.34 | 3 | 19 | 1 | 4 | 273-424 |
| CH | -1.72 | 1987 | 1305 | 0.13 | -8.0 | 4.2 | 0.06 | 6 | 56 | 0 | 0 | 273-423 |
| CH$_2$ | 0.70 | 2962 | 291 | < 0.001 | -8.43 | 0.90 | < 0.001 | 17 | 935 | 1 | 92 | 273-456 |
| CH$_3$ | 3.67 | 3683 | 557 | < 0.001 | -8.73 | 1.76 | < 0.001 | 33 | 1034 | 4 | 170 | 262-568 |
| C$_{ar}$[e] | -3.85 | -102 | 586 | 0.86 | 0.05 | 1.8 | 0.98 | 13 | 388 | 1 | 90 | 262-568 |
| CH$_{ar}$[e] | -0.65 | 1849 | 26 | < 0.001 | -4.16 | 0.07 | < 0.001 | 13 | 1940 | 1 | 450 | 262-568 |
| C=C | -10.23 | 9750 | 23970 | 0.68 | -34 | 80 | 0.67 | 3 | 59 | 1 | 6 | 273-361 |
| H[f] | 3.91 | -153 | 6566 | 0.98 | 2.3 | 22 | 0.92 | 6 | 246 | 2 | 30 | 273-361 |
| I(C-C)[g] | -1.01 | 6047 | 4279 | 0.16 | -19.2 | 13.9 | 0.17 | 5 | 46 | 0 | 0 | 273-353 |
| C=O[h] | -22.74 | 4520 | 1010 | < 0.001 | -4.0 | 3.1 | 0.20 | 19 | 332 | 3 | 34 | 265-453 |
| OH | -25.4 | 5094 | 1039 | < 0.001 | 0.2 | 3 | 0.96 | 29 | 480 | 3 | 48 | 273-375 |
| HCOO[i] | -15.33 | -1650 | 5960 | 0.78 | 14 | 20 | 0.48 | 6 | 62 | 1 | 12 | 272-364 |
| $Y^0$ | 7.95 | 0 | - | - | 0 | - | - | - | - | - | - | - |

[a]From Plyasunov et al. [243-247]

[b]Standard error

[c]Two-tailed p-values

[d]Cyclic (nonaromatic) group

[e]Aromatic carbon

[f]Hydrogen bound to alkene group

[g]Correction for nearest-neighbor interactions of two –CH$_3$ or –CH$_2$- groups attached to the benzene ring or to the cyclic ring for cis-isomers

[h]Ketone

[i]Formate

Efforts to expand the model to include esters and ethers were unsuccessful because the first-order contributions were not always adequate in modeling the behavior of compounds with functional groups [244-247]. Due to these limitations, a different model was pursued.

### 7.3.4 Second-Order Group Contribution Method

Plyasunov et al. [244-247] developed a second-order group contribution model due to the first-order limitations. A second-order method takes into account the nearest neighbor interactions for particular groups. This requires defining more groups than a first-order group contribution method. The group definitions as outlined by Domalski et al. [293] were used for parsing the compounds. Plyasunov et al. [244-247] only define four hydrocarbon second-order contributions. Additional hydrocarbon contributions were first established at 298.15 K before developing temperature-dependent contributions.

#### *7.3.4.1 Reference Value Additions*

The values of the four hydrocarbon groups defined by Plyasunov et al. [244-247] were used without modification. Values for four alkylbenzene groups were developed in this study. Accepted $k_H$ values at 298.15 K were found for 17 alkylbenzenes. Two of these compounds were randomly chosen for the validation set. The 15 training set compounds were divided into 10 subgroups. A 10-fold cross validation was performed as previously described. Only three of the four parameters could be determined in one of the iterations due to the learning model not being full rank. Of the remaining 9 iterations, the relative absolute standard deviation of the group contribution values did not exceed 5.6%. Overall parameters were determined using the full training set, and the model was applied to the validation set. The AAD of the overall training set was 18% and the AAD of the validation set was 14%.

An additional ether term was also developed, C-$(H)_3$(O), for a reference value at 298.15 K. A total of 7 compounds were found with this group. One of the compounds was randomly set aside for validation. A leave-one-out cross-validation was performed on the remaining 6 compounds (similar idea as the 10-fold cross-validation except each compound is a subset). The value of the group contribution did not change significantly during cross-validation (standard deviation of 2%). The AAD of the overall training set (6 compounds) was 21% and the AAD of the validation set (1 compound) was 1%. Table 7.8 is a summary of the second-order group contribution values for the prediction method at 298.15 K that were determined in this study and by Plyasunov et al. [244-247]. The table includes the number of compounds with each group (nC) and the number of times each group appeared in a set (nG).

#### *7.3.4.2 Temperature-Dependent Contributions*

A total of 31 (aliphatic and aromatic) hydrocarbons defined by the groups in Table 7.8 have temperature-dependent data. Four were randomly selected by subfamily (2 alkanes, 2 benzene derivatives) for validation. The training set of 27 compounds was divided into 10 groups for 10-fold cross-validation. Overall parameters were determined using the full training set. Results of the 10-fold cross-validation and overall method performance are summarized in Table 7.9 and shown in Figure 7.3.

Table 7.8: Summary of second-order group contributions for reference values at 298.15 K and 0.1 MPa

| | Training | | Validation | | $\Delta G^{\infty}_{hyd,i}$ | | |
|---|---|---|---|---|---|---|---|
| Group[a] | nC[b] | nG[c] | nC[b] | nG[c] | kJ/mol | SE[d] | p-value[e] |
| C-(H)$_2$(C)(Cb) | 6 | 6 | 0 | 0 | 1.02 | 0.31 | 0.007 |
| C-(H)$_3$(Cb) | 8 | 21 | 1 | 3 | 4.00 | 0.33 | < 0.0001 |
| Cb-(C)(Cb)$_2$ | 15 | 28 | 1 | 3 | -4.53 | 0.36 | < 0.0001 |
| Cb-(H)(Cb)$_2$ | 15 | 62 | 2 | 9 | -0.60 | 0.04 | < 0.0001 |
| C-(H)$_3$(O) | 6 | 7 | 1 | 1 | 3.48 | 0.11 | < 0.0001 |
| C-(H)$_3$(C)[f] | 7 | 8 | 0 | 0 | 3.72 | - | - |
| C-(H)$_2$(C)$_2$[f] | 5 | 18 | 0 | 0 | 0.68 | - | - |
| C-(H)(C)$_3$[f] | 1 | 1 | 0 | 0 | -1.93 | - | - |
| C-(C)$_4$[f] | 0 | 0 | 0 | 0 | -4.60 | - | - |
| [CH$_3$-CH$_2$-O-CH$_2$] corr[f,g] | - | - | - | - | -1.42 | - | - |
| [O-(CH$_2$)$_2$-O] corr[f,g] | - | - | - | - | 2.22 | - | - |
| C-(C)(H)$_2$(O)[f] | - | - | - | - | 0.77 | - | - |
| C-(C)$_2$(H)(O) alcohol[f] | - | - | - | - | -1.64 | - | - |
| C-(C)$_2$(H)(O) ester[f] | - | - | - | - | -1.46 | - | - |
| C-(C)$_2$(H)(O) ether[f] | - | - | - | - | -2.82 | - | - |
| C-(C)$_3$(O) alcohol[f] | - | - | - | - | -4.58 | - | - |
| C-(C)$_3$(O) ester[f] | - | - | - | - | -2.58 | - | - |
| C-(C)$_3$(O) ether[f] | - | - | - | - | -7.77 | - | - |
| C-(CO)(C)$_3$[f] | - | - | - | - | -2.50 | - | - |
| C-(CO)(H)(C)$_2$[f] | - | - | - | - | -0.88 | - | - |
| C-(CO)(H)$_2$(C)[f] | - | - | - | - | 1.15 | - | - |
| CO-(C)$_2$[f] | - | - | - | - | -23.46 | - | - |
| COO-(C)$_2$[f] | - | - | - | - | -20.53 | - | - |
| HCOO-(C)[f] | - | - | - | - | -15.43 | - | - |
| O-(C)(H)[f] | - | - | - | - | -25.46 | - | - |
| O-(C)$_2$[f] | - | - | - | - | -15.52 | - | - |
| $Y^0$ [f] | - | - | - | - | 7.95 | - | - |

[a] Cb is an aromatic carbon (benzene)
[b] nC is the number of compounds with the group
[c] nG is the number of times the group appeared in the set
[d] Standard error
[e] Two-tailed p-value
[f] Determined by Plyasunov et al. [244-247]
[g] ether corrections; used in addition to group contributions

Table 7.9: Performance summary of the second-order temperature-dependent group contribution method for alkylbenzenes

| Set | #Compounds | AAD | $R^2$ | 10-Fold Cross-Validation | Avg. AAD | Avg. $R^2$ |
|---|---|---|---|---|---|---|
| Training | 27 | 10% | 0.998 | Learning | 10% | 0.998 |
| | | | | Prediction | 19% | 0.950 |
| Validation | 4 | 14% | 0.997 | - | - | - |

Temperature-dependent parameters were then determined for functional groups using the hydrocarbon backbone. In order for the model to be full rank, either structural groups had to be redefined or group contribution values had to be defined. There are three carbon groups associated with the O-(C)(H) group (hydroxyl group). The hydroxyl group will always be found in a 1:1 ratio with these three groups, so the hydroxyl group cannot be considered an independent variable. The groups could be redefined to include the hydroxyl group which would cause the model to be full rank. The groups as defined by Plyasunov et al. [244-247] and possible new group definitions are given in Table 7.10. However, as originally defined the C-(C)$(H)_2$(O) group applies to ethers and esters in addition to alcohols, so an additional group would have to be added for ethers and esters if these new group definitions were used. In order to still use the original group definitions, the hydroxyl contributions were defined as 0. This is essentially treating the carbon groups as if they were the new groups given in Table 7.10 without formally redefining them. The C-(C)$(H)_2$(O) group is then still applicable for other chemical families.

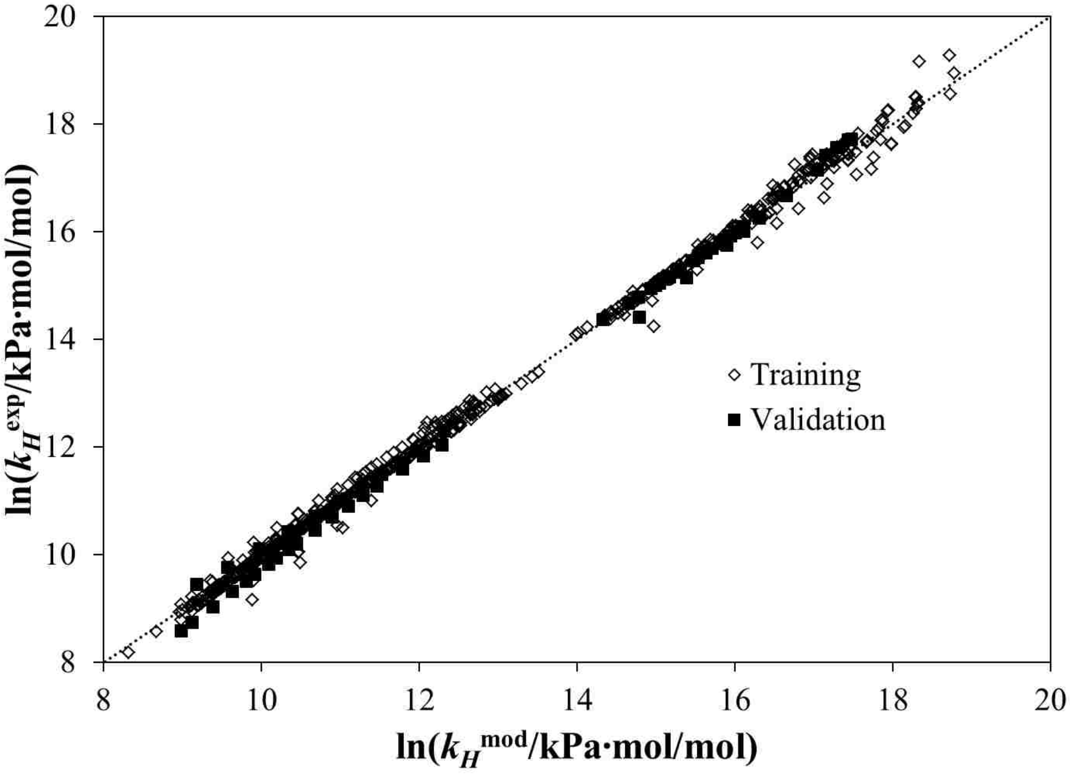

Figure 7.3: Plot of experimental versus model values for the second-order temperature-dependent group contribution method for alkylbenzenes and alkanes

Table 7.10 Second-order alcohol groups

| Plyasunov et al. [244-247] group | "New" group |
|---|---|
| C-(C)(H)$_2$(O) | C[OH]-(C)(H)$_2$[a] |
| C-(C)$_2$(H)(O) alcohol | C[OH]-(C)$_2$(H) |
| C-(C)$_3$(O) alcohol | C[OH]-(C)$_3$ |
| O-(C)(H) | NA |

[a]Only for alcohols. Group treated as original definition for other compounds

If a group was only represented in 1 or 2 compounds, the compounds were added to the training set. The remaining compounds were divided into subsets (COO, CH$_3$O, COOH, CO, OH, and O), and compounds were randomly chosen from each subset to ensure multiple groups were represented in the validation set. The training and validation sets contained data for 83 and

11 compounds, respectively. During model development, it was discovered that the model showed a predictable bias. Figure 7.4 shows the natural log of the ratio of the experimental versus model values normalized by the reference value. Also shown in the figure is the line that corresponds to a perfect model. A correction factor was added to the model to improve the results.

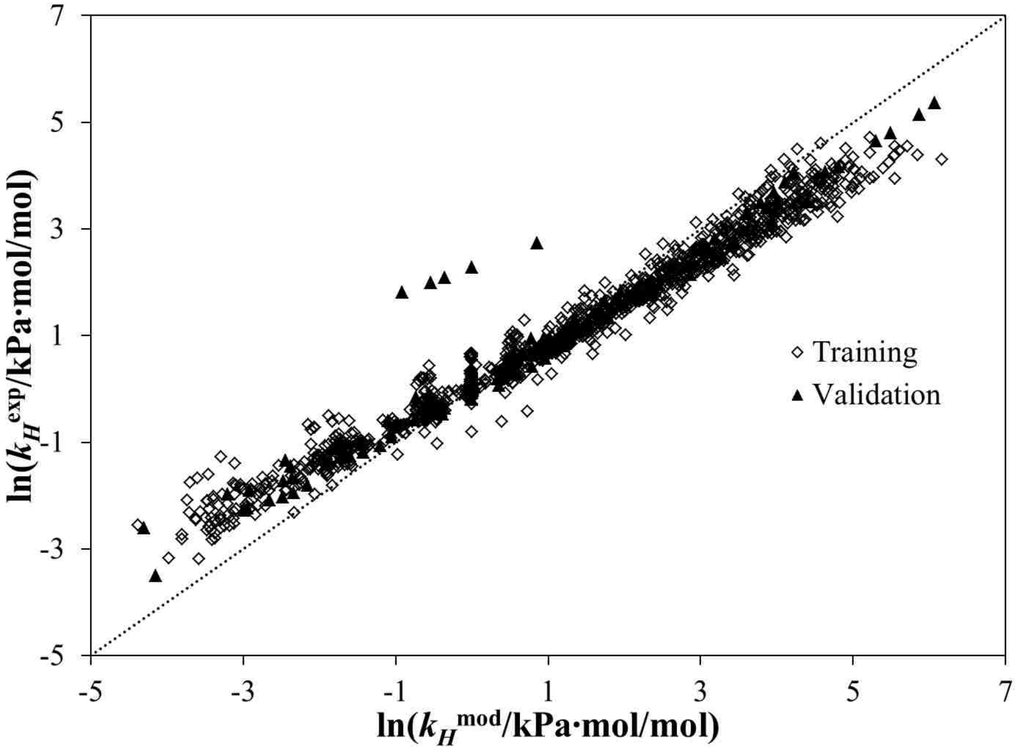

Figure 7.4: Initial second-order group contribution model performance for functional groups

The correction factor was obtained by determining the slope, *D*, of the training set values as plotted in Figure 7.4. The modified model is then given by:

$$\ln\left(\frac{k_H}{k_{H,ref}}\right) = D\left[\left(\sum_i B_i n_i\right)\left(\frac{1}{T_{ref}} - \frac{1}{T}\right) + \left(\sum_i C_i n_i\right)\left(\ln\left(\frac{T}{T_{ref}}\right)\right)\right]. \qquad 7.7$$

The correction factor is only necessary for alcohols, esters, ethers, and ketones. For hydrocarbons, *D* equals unity. Figure 7.5 shows the corrected natural log of the ratio of the experimental versus model values normalized by the reference value. The outliers in Figure 7.4 and Figure 7.5 are data points for 2-butoxyethanol which is a multifunctional compound. Plyasunov et al. [247] found it necessary to provide a correction for diethers ([O-$(CH_2)_2$-O]. 2-Butoxyethanol has a similar structure except that one ether group is replaced by a hydroxyl group. A correction factor was not added in this study due to the limited amount of data. However, the data from this compound suggest that correction factors may be necessary for multifunctional compounds.

The training set was divided into 10 subgroups for 10-fold cross-validation. With three of the folds, the learning sets were not full rank so parameters could not be determined. The results of the remaining seven iterations were averaged for the cross-validation statistics. Overall parameters were determined using the full training set. The model was then applied to the validation set. Results of the 10-fold cross-validation and overall method performance are summarized in Table 7.11. Results are shown in Figure 7.6.

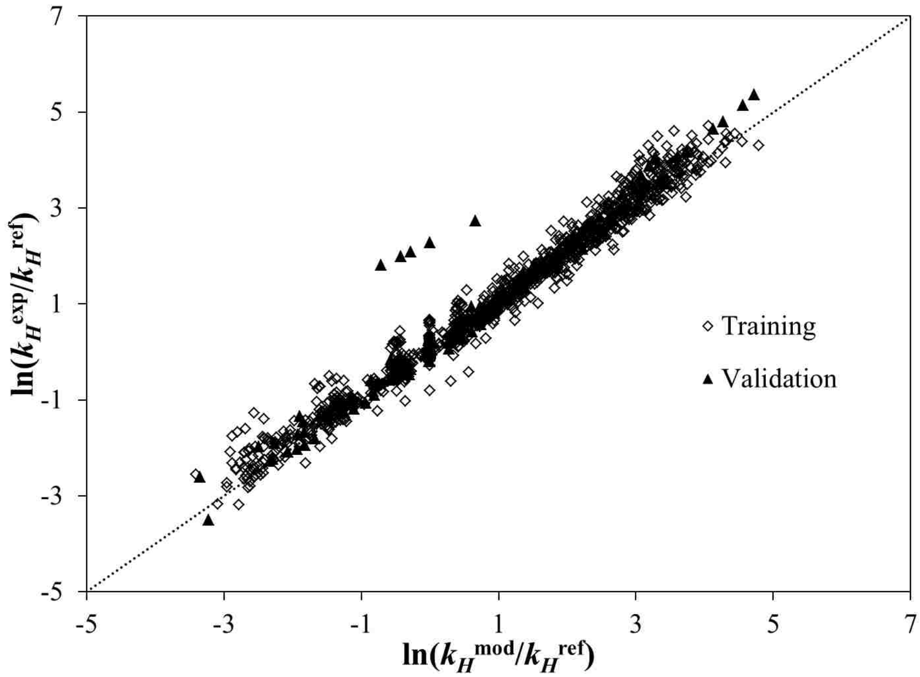

Figure 7.5: Corrected second-order group contribution model performance for functional groups

Table 7.11: Summary of performance for second-order temperature-dependent group contribution method for esters, ethers, ketones, and alcohols

| Set | #Compounds | AAD | $R^2$ | 10-Fold Cross-Validation[a] | Avg. AAD | Avg. $R^2$ |
|---|---|---|---|---|---|---|
| Training | 83 | 17% | 0.987 | Learning | 18% | 0.986 |
| | | | | Prediction | 21% | 0.982 |
| Validation | 11 | 19% | 0.970 | - | - | - |

[a] Only includes results of the seven iterations that were full rank

The second-order group contribution method works slightly better for hydrocarbons than compounds with functional groups. This is not surprising due to the increased complexity of the compound structures. In addition, there are typically less temperature-dependent data available for the compounds with functional groups, and the data generally had higher experimental uncertainties.

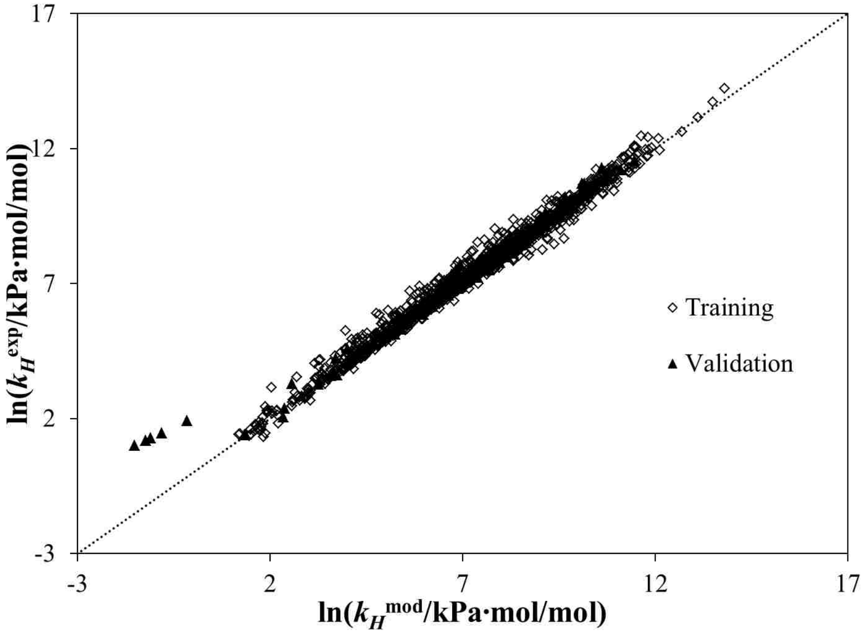

Figure 7.6: Plot of experimental versus model values for the second-order temperature-dependent group contribution method for esters, ethers, ketones, and alcohols

All of the temperature-dependent groups developed in the two regressions (hydrocarbon and functional groups) and the coefficient standard errors (SE) and two-tailed p-values are summarized in Table 7.12. Only the first four hydrocarbon groups were used in the functional group regression. The table also includes the number of times a group appeared in a compound (nC) and the number of times a group appeared in all of the temperature-dependent data (nG) in the training and validation sets for each regression. The minimum and maximum temperatures of the data corresponding to each group found in the training and validation sets is also included. The groups with the smallest amount of data typically have the largest standard errors and p-values. The second-order correction factor is summarized in Table 7.13. Sample calculations are included in Appendix D.

Table 7.12: Summary of second-order temperature-dependent model values

| Group | $B_i$ | | | $C_i$ | | | Training | | Validation | | Temp. Range |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | Value/K | SE | p-value | Value | SE | p-value | nC | nG | nC | nG | K |
| Hydrocarbon Regression | | | | | | | | | | | |
| C-(C)$_4$ | -5451 | 2205 | 0.01 | 13.2 | 7.1 | 0.06 | 4 | 23 | 0 | 0 | 273-424 |
| C-(H)(C)$_3$ | -4267 | 1166 | 0.0003 | 11.8 | 3.8 | 0.002 | 5 | 45 | 1 | 11 | 273-423 |
| C-(H)$_2$(C)$_2$ | 868 | 292 | 0.003 | -1.89 | 0.90 | 0.04 | 13 | 830 | 3 | 56 | 273-456 |
| C-(H)$_3$(C) | 6820 | 542 | < 0.0001 | -18.6 | 1.7 | < 0.0001 | 19 | 645 | 3 | 90 | 273-456 |
| C-(H)$_2$(C)(Cb) | 19962 | 33762 | 0.55 | -65 | 111 | 0.56 | 4 | 115 | 1 | 11 | 273-373 |
| C-(H)$_3$(Cb) | 16423 | 33753 | 0.63 | -52 | 111 | 0.64 | 7 | 303 | 1 | 38 | 262-568 |
| Cb-(C)(Cb)$_2$ | -13358 | 33753 | 0.69 | 45 | 111 | 0.69 | 12 | 423 | 2 | 49 | 262-568 |
| Cb-(H)(Cb)$_2$ | 1870 | 20 | < 0.0001 | -4.28 | 0.06 | < 0.0001 | 13 | 2229 | 2 | 131 | 262-568 |
| $Y^0$ | 0 | - | - | 0 | - | - | - | - | - | - | - |
| Functional Group Regression | | | | | | | | | | | |
| [CH$_3$-CH$_2$-O-CH$_2$] corr[a] | 1106 | 5853 | 0.85 | -6 | 19 | 0.76 | 2 | 35 | 0 | 0 | 269-364 |
| [O-(CH$_2$)$_2$-O] corr[a] | -26034 | 17351 | 0.14 | 72 | 56 | 0.20 | 1 | 11 | 0 | 0 | 273-373 |
| C-(C)(H)$_2$(O) | 22467 | 1574 | < 0.0001 | -49.8 | 4.9 | < 0.0001 | 39 | 608 | 7 | 103 | 269-375 |
| C-(C)$_2$(H)(O) alcohol | 19591 | 994 | < 0.0001 | -39.3 | 3.1 | < 0.0001 | 11 | 174 | 2 | 20 | 273-373 |
| C-(C)$_2$(H)(O) ester | 18533 | 6657 | 0.006 | -38 | 21 | 0.07 | 2 | 11 | 0 | 0 | 273-364 |
| C-(C)$_2$(H)(O) ether | 12226 | 5167 | 0.02 | -15 | 17 | 0.37 | 1 | 40 | 0 | 0 | 273-334 |
| C-(C)$_3$(O) alcohol | 18816 | 2525 | < 0.0001 | -36.8 | 7.9 | < 0.0001 | 3 | 42 | 0 | 0 | 273-371 |
| C-(C)$_3$(O) ester | 34714 | 6219 | < 0.0001 | -90 | 20 | < 0.0001 | 2 | 21 | 0 | 0 | 273-354 |
| C-(C)$_3$(O) ether | 12359 | 9442 | 0.19 | -15 | 30 | 0.62 | 3 | 72 | 1 | 9 | 273-363 |
| C-(CO)(C)$_3$ | -7084 | 15452 | 0.65 | 25 | 49 | 0.61 | 1 | 10 | 0 | 0 | 273-364 |
| C-(CO)(H)(C)$_2$ | -14006 | 4324 | 0.001 | 46 | 14 | 0.0007 | 3 | 28 | 0 | 0 | 273-364 |
| C-(CO)(H)$_2$(C) | -9550 | 2434 | < 0.0001 | 32.2 | 7.6 | < 0.0001 | 12 | 128 | 4 | 42 | 273-364 |
| CO-(C)$_2$ | 17819 | 805 | < 0.0001 | -37.8 | 2.5 | < 0.0001 | 19 | 306 | 1 | 13 | 265-453 |
| COO-(C)$_2$ | -5096 | 2902 | 0.08 | 13 | 9 | 0.17 | 21 | 259 | 4 | 42 | 273-365 |
| HCOO-(C) | 1855 | 5873 | 0.75 | -14 | 19 | 0.47 | 6 | 50 | 1 | 14 | 272-364 |
| O-(C)(H) | 0 | - | - | 0 | - | - | 27 | 425 | 4 | 54 | 273-375 |
| O-(C)$_2$ | -29379 | 5765 | < 0.0001 | 68.9 | 18.7 | 0.0002 | 9 | 173 | 2 | 14 | 269-373 |
| C-(H)$_3$(O) | 28004 | 7327 | 0.0001 | -69.9 | 23.3 | 0.003 | 6 | 112 | 1 | 6 | 273-373 |

[a] ether corrections; used in addition to group contributions

Table 7.13: Second-order method correction factor

| Chemical Families | *D* | |
|---|---|---|
| | Value | SE |
| Hydrocarbons | 1 | - |
| Alcohols, Ketones, Esters, Ethers | 0.7758 | 0.0034 |

### 7.3.5 Method Application Summary

The general procedure required to use the first- and second-order bond contribution methods of this study are described in the following steps.

1. Calculate $k_{H,ref}$ using Equation 7.2 and the $\Delta G^{\infty}_{hyd}$ contributions listed in
2. Table 7.7 for the first-order method and Table 7.8 for the second-order method.
3. Calculate coefficients *B* and *C* using the group contribution values listed in
4. Table 7.7 for the first-order method and Table 7.12 for the second-order method.
5. Determine coefficient *D* using Table 7.13 if using the second-order method.
6. Determine the final equation by combining the coefficients and reference value using Equation 7.1 for the first-order method and Equation 7.7 for the second-order method.

### 7.3.6 Method Comparison and Recommendations

The methods of this study were compared with the literature methods using data from 144 compounds used in the first- and second-order method development. The reference point used in the Lau et al. [39] and Kühne et al. [285] methods is the recommended Smoothed or Experimental value at 298.15 K from this study. The results are summarized in Table 7.14.

The first- and second-order methods from this study are comparable to the methods of Lau et al. [39] and better than the method of Kühne et al. [285] for hydrocarbons. However, in general the methods of Kühne et al. [285] and Lau et al. [39] (when applicable) are more accurate for compounds with functional groups. This is partially due to the fact that these methods used an experimental value as a reference point instead of a predicted value. The first-order group contribution method from this study is recommended for hydrocarbons, alcohols, ketones, and formats where the functional group is not directly attached to a benzene ring. It is easier to use than the Lau et al. [39] methods because it does not require an additional prediction method or experimental value. The Kühne et al. [285] method is recommended for compounds with functional groups over a limited temperature range that have reliable reference values. The second-order group contribution method developed in this study is recommended for compounds without a reliable experimental reference point.

Table 7.14: Comparison of methods from this study with existing methods

| Method | Kühne AAD% | nC | Lau GCM AAD% | nC | Lau BCM AAD% | nC | This study $1^{st}$ order AAD% | nC | This study $2^{nd}$ order AAD% | nC |
|---|---|---|---|---|---|---|---|---|---|---|
| Overall | 49.9 | 144 | 18.6 | 101 | 11.6 | 50 | 24.2 | 108 | 24.5 | 125 |
| 1-Alkenes | 12.2 | 2 | 21.0 | 2 | - | - | 7.4 | 2 | - | - |
| Acetates | 14.9 | 10 | - | - | - | - | - | - | 26.3 | 10 |
| Aliphatic ethers | 16.9 | 9 | - | - | - | - | - | - | 25.7 | 9 |
| Alkylcyclohexanes | 258.4 | 4 | 11.1 | 4 | - | - | 48.0 | 4 | - | - |
| Cycloaliphatic alcohols | 9.5 | 1 | 7.0 | 1 | - | - | 37.7 | 1 | - | - |
| Cycloalkanes | 21.8 | 4 | 14.6 | 4 | - | - | 52.7 | 4 | - | - |
| Cycloalkenes | 8.1 | 3 | 14.7 | 3 | - | - | 40.6 | 3 | - | - |
| Dialkenes | 10.8 | 1 | 7.4 | 1 | - | - | 65.6 | 1 | - | - |
| Dimethylalkanes | 159.3 | 4 | 9.8 | 4 | 11.2 | 4 | 23.9 | 4 | 22.8 | 4 |
| Formates | 14.9 | 7 | - | - | - | - | 20.9 | 7 | 33.0 | 7 |
| Ketones | 35.8 | 22 | 38.1 | 22 | 11.7 | 20 | 30.2 | 22 | 28.3 | 21 |
| Methylalkanes | 67.4 | 2 | 13.8 | 2 | 13.3 | 2 | 14.1 | 2 | 14.8 | 2 |
| Methylalkenes | 6.3 | 2 | 45.1 | 2 | - | - | 7.5 | 2 | - | - |
| *n*-Alcohols | 29.7 | 10 | 14.5 | 10 | - | - | 21.5 | 10 | 17.6 | 10 |
| *n*-Alkanes | 172.9 | 8 | 14.1 | 8 | 14.5 | 8 | 16.1 | 8 | 15.6 | 8 |
| *n*-Alkylbenzenes | 21.2 | 7 | 8.9 | 7 | 8.7 | 7 | 10.1 | 7 | 8.8 | 7 |
| Other aliphatic alcohols | 20.5 | 21 | 11.5 | 21 | - | - | 22.1 | 21 | 22.7 | 21 |
| Other alkanes | 28.7 | 1 | 21.6 | 1 | 4.4 | 1 | 20.3 | 1 | 16.7 | 1 |
| Other alkylbenzenes | 163.2 | 8 | 10.9 | 8 | 11.4 | 8 | 14.6 | 8 | 29.8 | 8 |
| Other ethers/diethers | 13.1 | 1 | - | - | - | - | - |  | 35.1 | 1 |
| Other monoaromatics | 6.2 | 1 | 6.9 | 1 | - | - | 6.0 | 1 | - | - |
| Other polyfunctional C, H, O | 10.3 | 1 | - | - | - | - | - | - | 89.7 | 1 |
| Other saturated aliphatic esters | 27.6 | 2 | - | - | - | - | - | - | 37.9 | 2 |
| Propionates and butyrates | 26.4 | 13 | - | - | - | - | - | - | 25.5 | 13 |
| < 3% | 15.4 | 8 | 13.4 | 6 | 5.5 | 4 | 5.6 | 6 | 11.6 | 7 |
| < 5% | 41.4 | 25 | 7.5 | 21 | 7.1 | 9 | 16.6 | 22 | 17.7 | 21 |
| < 10% | 43.5 | 71 | 12.1 | 53 | 9.8 | 29 | 19.3 | 56 | 19.5 | 66 |
| < 25% | 52.1 | 76 | 31.3 | 51 | 20.1 | 25 | 36.4 | 54 | 30.7 | 66 |
| < 50% | 58.0 | 29 | 43.5 | 23 | 45.9 | 13 | 46.9 | 23 | 46.7 | 27 |
| < 100% | 68.3 | 15 | 71.1 | 11 | 75.4 | 8 | 88.0 | 11 | 71.4 | 13 |

# 8 Summary

A database containing recommended values for Henry's law constants, infinite dilution activity coefficients and solubility data of industrially important chemicals has been compiled for aqueous systems. These properties are important in predicting the fate and transport of chemicals in the environment. The structure of this database is compatible with the existing DIPPR® 801 database and DIADEM interface. Recommendations have been provided for 498 compounds for at least one of the properties.

Thermodynamic relationships, chemical family trends, and predicted values were important data analysis tools. Data from the various properties were related to each other using thermodynamic relationships and reliable DIPPR® 801 pure component property values. For hydrophobic compounds, the data from the three properties were combined to obtain recommendations. In instances where the data could not be combined, the thermodynamic relationships were helpful in identifying the best datasets. Chemical family plots were used with temperature-dependent and single-temperature data to check for consistency within chemical families and to select the best data. Predicted values were used to select the best datasets when there were discrepancies in the literature data. Notes in the database provide information about the procedure and data used to provide recommendations for each compound and property.

Henry's law constants were measured for seven compounds at various temperatures and atmospheric pressure using the inert gas stripping method. Two of these compounds were used to validate the experimental method, and good agreement was obtained between results from this study and literature values. The remaining compounds were chosen to clarify discrepancies between literature values or to provide values for compounds that have not been measured. Infinite dilution activity coefficients were determined for each compound. A fugacity ratio was required to determine infinite dilution activity coefficients for the solid solutes. It was obtained from the heats of fusion and the liquid and solid heat capacities for the pure solutes as obtained from the DIPPR® 801 database. The experimental work was published [294].

A first-order temperature-dependent group contribution method was developed using the method of Plyasunov et al. [243] as a reference point. The method works for hydrocarbons, alcohols, ketones, and formats where none of the functional groups are directly attached to a benzene ring. Attempts to add group contributions for ethers and esters were unsuccessful. A second-order temperature-dependent group contribution method was developed using the groups defined by Plyasunov et al. [244-247]. Additional second-order hydrocarbon groups were first defined at the reference condition of 298.15 K and 100 kPa before developing temperature-dependent parameters. The method is applicable for hydrocarbons, esters, ethers, ketones, and alcohols. The first-order group contribution method from this study is recommended when applicable. It is easier to use than the Lau et al. [39] methods because it does not require an additional prediction method or experimental value. The Kühne et al. method [285] is recommended for esters and ethers below 353 K when a reliable experimental reference value is available. The second-order group contribution method developed in this study is recommended for esters and ethers when a reliable experimental value is not available for a reference point.

## 8.1 Recommendations for Future Work

The 801E database could be expanded to include additional properties. As mentioned in Section 2.1.3, derivative properties ($\Delta H_{hyd}^{\infty}$, $\Delta Cp_{hyd}^{\infty}$, and $V^{\infty}$) are thermodynamically related to $k_H$. These properties could be added to the database to further aid in the designation of recommended values and the development of prediction methods.

The current database does not take into account the effects of pressure which are significant for gases. Because of this, API recommendations were accepted (see Section 4.5). The database could be modified to include pressure as a dependent variable. This would allow data at intermediate and high pressures to be included. The unit conversions could be modified in order to take into account non-idealities due to high temperatures and pressures. More data at high temperatures and pressures could also be included for compounds that are liquids and solids.

Although SOLC data were included in the database, no efforts were made to provide recommended values for this property. In the future, SOLC and $x_i^{aq}$ data could be analyzed simultaneously to obtain the entire solubility curves for compounds with critical solution temperatures.

Further temperature-dependent $k_H$ experiments could be performed to continue measuring compounds with discrepancies in the literature and/or missing literature data. If temperature-dependent regressions have been assigned high uncertainties, then the available data have significant noise. Additional measurements could provide a better regression. In addition, measurements could be performed for compounds with interesting chemical family trends (i.e. cycloalkanes, cycloalkenes, *n*-alkanes) to provide further insights into the trends. More data would also be useful for compounds with multiple functional groups.

Additional second-order group contribution reference values can be added to the prediction method developed in this study to broaden the chemical applicability. Prediction methods have the largest errors for compounds with multiple functional groups. Unfortunately, limited data are available for multifunctional compounds. As mentioned, additional experimental work could provide more data for multifunctional compounds allowing for the development of better prediction methods.

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# Appendix A. Experimental Method Details

Table A.1: $x_i^{aq}$ experimental methods

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Column elution method [1, 2] | Water is used to elute a substance that is coated on an inert carrier material (glass beads, silica gel, sand, etc.) contained in a small column. Solubility is determined when the mass concentration of the exiting stream becomes constant with time. | Good method for $x_i^{aq} < 10^{-2}$ g/L. Not to be used for volatile chemicals because they can evaporate with the solvent during loading of the carrier material |
| HPLC correlation [3, 4] | Chemicals injected into an HPLC column have various retention times. Reference values are used to develop a relationship between the property ($x_i^{aq}$) and retention time. This relationship is used to find the property of other compounds based on retention time. | Reference substance is needed, so this is sometimes considered an estimation method. This method should not be used for strong acids and bases, metal complexes, or compounds that react with either the eluent or column packing. |
| Shake flask method [1] or batch contacting [5] or equilibrium cell | An excess amount of solute is added to a flask and shaken or vigorously stirred. It is then centrifuged or allowed to settle, and the concentration is determined in the aqueous phase (or in both phases) using an analytical method (ex. GC, HPLC, UV, etc.). | Good method for $x_i^{aq} > 10^{-2}$ g/L. Problems that can arise with less soluble substances include: incomplete equilibration, dispersion rather than dissolution if the solute is a solid, suspension of microcrystals in solution, adsorptive losses on equipment surfaces, and interference from impurity and/or water signals. This method should not be used for volatile chemicals which tend to be less soluble. |
| Radiometric method [6]<br>(similar to shake flask method) | Radioagent is dissolved in organic solvent before pure water is added. Mixture is shaken vigorously. Some organic solvent dissolves in water, which causes a volume reduction of the organic phase. The radioagent does not dissolve in water. The specific activities of the radioagent are measured initially and finally in order to estimate the decreased volume of the organic phase. | |

Table A.1: $x_i^{aq}$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Generator column or dynamic coupled column liquid chromatographic technique [7-12] | Water is pumped through the generator column that is packed with a solid support coated with the test compound to produce a saturated aqueous solution. The compound is then extracted from the saturated solution onto an extractor column. It is then eluted with a solvent/water mixture and analyzed with HPLC or GC. The water solubility is the concentration of the compound in the generator column effluent. (similar to column elution method) | This method avoids errors that could result from sorption on glassware and the presence of colloids when measuring small concentrations. Recommended range is 1 ppb-500 ppm. |
| Nephelometric or turbidity method [13] | Several dilutions are made of a stable suspension of known concentration. A plot of concentration verses turbidity produces a line. $x_i^{aq}$ is the concentration at 0 turbidity, and it can be estimated through a linear regression of the turbidity data. | This method cannot distinguish between solute and impurities. Recommended for $x_i^{aq} > 10^{-3}$ g/L if the solute forms stable suspensions in water. |
| Slow stir method [13] | The sample is dissolved in a volatile solvent. This solution is deposited on the walls (not the bottom) of a glass container, and the solvent is evaporated using nitrogen. Water and a magnetic stir bar are added, and the system is mixed until equilibrium is reached. The concentration in the aqueous phase is then determined using an appropriate analytical technique. | Recommended for $x_i^{aq} < 10^{-3}$ g/L. This method avoids emulsions. |
| Gas solubility methods | The apparatus is a complex system that uses manometers and multiple vessels. A known mass of solvent is used. Equilibration can be accomplished through stirring, bubbling, shaking, or static contact. The final concentration can be determined by mass, pressure, volume, or an analytical technique. | |
| Thermostatic (for SOLC) [14] | In various solvents, the solubility of silver perchlorate increases in the presence of trace amounts of water. The solubility behavior can be used to determine how much water is present. | |
| Vapor Saturation [15] | Solvent is equilibrated with solute vapor. | |
| Residue volume or volumetric method or absorbed volume [16, 17] | An excess of solute is added and the mixture is centrifuged. The residue of solute is then measured volumetrically. The data is then plotted as grams of solute added vs. volume of undissolved residue. The value at zero volume of undissolved residue is then extrapolated. | |
| Synthetic method [17] | Weighed quantities of solute and solvent are sealed up together. The temperature at which turbidity appears/disappears is determined in a temperature bath. | This cannot distinguish between solute and impurities. |
| Multiple equilibration [18] | See Table A.2 for description. | |
| Dialysis tubing method [19] | Dialysis tubing containing pure water is knotted on one end, connected to glass tubing on the other end, and sealed with a plastic cap. This tubing is then put in a test tube containing solute. Injections are taken and analyzed with a GC. | |

Table A.1: $x_i^{aq}$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Surface tension method [20] | Surface tension is measured by the drop weight method. From the surface tension and the logarithm of the concentration, the saturation points are determined. | |
| Solute vapor absorption [21] | This method is similar to the EXPSAT method (see Table A.2). Inert gas is saturated with solute and solvent and then bubbled through solvent until the solvent is saturated with solute. | |
| Cloud point or isothermal method | Solute is added to solvent until a precipitate is observed. | |
| Equilibrium cell with gas agitation [22] | Excess solute is added to the equilibrium cell. Mixing is accomplished by bubbling $N_2$ through the cell. Flow is stopped and layers are allowed to separate and equilibrate. Concentration is determined using an analytical method. | |
| Isopiestic method [23] | See Table A.3. | |
| Laser Multiphoton Ionization [24] | Combines microdroplet sampling and multiphoton ionization-based fast-conductivity techniques. At the onset of equilibrium solubility, a sharp increase in the detected photocharges is recorded. | |
| Supersaturation [25] | Solute is dissolved in water at an elevated temperature and brought down to temperature of interest | |
| Static Cell [26] | Solute and solvent are allowed to equilibrate without shaking or stirring. | |

Table A.2: $k_H$ experimental methods

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Single equilibration [27] or equilibrium cell [28] | Solute and solvent are equilibrated in the liquid and vapor phases in a single cell. Concentration is measured in one or both phases. If only one phase is measured, the concentration in the other phase is calculated using a mass balance. This could be used as a general description for some of the methods described below. | This method is good for compounds with high vapor pressures and $x_i^{aq}$s [29, 30]. For compounds with low $x_i^{aq}$s and vapor pressures, it is difficult to determine the concentrations in either phase using analytical techniques. Other methods are preferred that utilize relative changes in detector response. |
| Internal standard | A dilute solution is made with two compounds, one of which has a known $k_H$. The solution is equilibrated with air, and concentrations are determined. Ratio of $k_H$ values is related to the ratio of peak areas. (similar to RGLC method for $\gamma_i^{\infty}$) | |

## Table A.2: $k_H$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Headspace solid-phase microextraction (SPME) [31, 32] | This is a single equilibration method that uses SPME as the analytical technique. | The SPME fiber must be calibrated in the standard gas atmosphere at a temperature and air humidity identical to those in the experiment. |
| Multiple Equilibration Technique [27, 33] or Indirect HGLC | A liquid sample with known volume and concentration is introduced into a variable volume vessel such as a syringe. The system is allowed to equilibrate with air. One of the phases is analyzed, and then the air is removed. The same amount of air is added to the vessel again and allowed to equilibrate. The selected phase is analyzed. This process can be repeated until the solute is undetectable. A plot of the log of the concentration in the gas phase verses the number of equilibrations produces a straight line. $k_H$ is related to the slope. | The $k_H$ error is reduced as the number of equilibrations increases and by using a larger gas/liquid volume ratio. This requires relatively large initial aqueous concentrations so that the concentration is still detectable after multiple equilibrations. |
| Headspace multiple-injection interrupted-flow (MIIF) technique [34, 35] | The first part of this method is like the $x_i^{aq}$ shake flask method. MIIF is an analytical headspace technique. Vapor removal in a closed system disturbs the equilibrium. Vapor samples are taken at known times, and a linear extrapolation of the GC response is used to determine the GC response at equilibrium. This is a modified method of Massaldi and King [36]. | Solutes must have appreciable vapor pressures. |
| Equilibrium Partitioning in Closed Systems (EPICS) [37] and modified EPICS [38] | Known masses are added to two systems of different volumes at the same temperature, and $k_H$ is determined from the ratio of the concentrations in one phase. The original EPICS calculations assumed that equal masses of solute were added to each container, but the modified EPICS only requires the relative masses to be known. If a stock solution is made, the concentration does not need to be known, only the relative masses added to each container. | The systems must be at the same temperature, and they must be allowed to equilibrate before measurement. The technique has the maximum sensitivity when one system has a low liquid volume and the other a high. Adsorption can be a problem [39]. A recommended range is $0.1 \leq k_H$ (unitless molar concentration basis) $\leq 1$ with a possible precision of 5% [40]. |
| Variable headspace or static headspace or phase ratio variation method [40, 41] | The relative air concentration is measured from aliquots of the same solution in multiple containers having different headspace-to-liquid ratios. Plots of the reciprocal of the GC peak area verses headspace-to-liquid volume ratios results in a linear plot. The slope and y-intercept are related to $k_H$. (similar to EPICS method) | Neither the exact concentrations of the compound or its matrix need to be known. This method is applicable for volatile and semivolatile organic compounds. This method can handle smaller liquid-phase loadings than EPICS which makes it work in lower regions (around 0.001 unitless molar concentration basis). |

Table A.2: $k_H$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Batch air stripping [30] or inert gas stripping or gas stripping or air stripping or exponential dilutor method | A dilute solution is stripped using an inert gas (usually $N_2$). The change in concentration with time is related to $k_H$. Some experiments first saturate the stripping gas with water. There are many variations of this method. The original equation has been expanded upon by multiple authors to include various corrections. Some authors take into account different corrections while others do not. | When compared to the single equilibration method, adsorption is less likely to be an issue due to the dynamic principle and turbulent conditions [39]. Absolute detector response is unimportant; it just needs to be linear [42]. It can be difficult to determine if equilibrium is reached [37] . The depth/height of the column can be increased. If the value does not change, then equilibrium was reached. However, a taller tower makes it harder to ensure complete mixing. Equilibrium can be verified by changing the flow rate of the stripping gas and seeing if $k_H$ remains constant [43]. A range of system volumes and purge gas flow rates can also be used to verify the assumptions of complete mixing and equilibrium [44]. Non-equilibrium leads to biased results [27, 39]. This method works for chemicals with low solubilities and vapor pressures [29, 45], but problems can arise if the volatility is too low because it is difficult to detect a change in concentration after air stripping [44]. It is a good method for systems with a high limiting relative volatility and involatile solvents [46]. Bias has been reported for this method for semivolatile organic chemicals[47]. The authors claim there can be significant absorption on the surface of the bubbles. When they pop on the surface, they release excess chemical into the headspace. Recommended ranges are $0.0001 < k_H$ (unitless molar concentration basis) $<1$[31]; relative volatility > 1000 [48]; 10 kPa $< k_H < 10^5$ kPa and $P_2^{sat} < 50$ kPa [40] with 1% uncertainty possible in this range. The diameter of the bubble should be below 1 mm, and they should not coalesce [40, 49] A good relative elution rate is 0.01 $min^{-1}$ or lower. Minimize the vapor space, and use as dilute a solution as possible. |
| EXPSAT (exponential saturator)[50, 51] | Contaminated air/$N_2$ (gas first saturated with solute) is bubbled through water to resemble what happens in atmosphere. | An advantage over gas stripping is that dissolution of hydrophobic compound in water to make dilute solution is not required [40]. Recommended ranges: $500 < \gamma_i^\infty < 10^5$ or 1 MPa $< k_H <$ 100 MPa with precision possible of 1-2%. |
| Modified gas stripping[52] | Differences between this and inert gas stripping are that chemical is introduced into stripping cell using a separate loop. Solute is in a separate flask. The line between the flask and stripping cell is "vacuumed". Line is opened and water saturated carrier is used to carry solute into cell (similar idea to EXPSAT). The concentration is monitored real time. | This is faster than the inert gas stripping method. This can be applied to a broader range of compounds than normal gas stripping. |

## Table A.2: $k_H$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Purge and trap[53] or gas sparging [54] or dynamic equilibrium system [55] | An inert gas is bubbled through a purge chamber. The exiting solute is deposited on a cooled trap or cartridge. The trap is then heated in order to inject the solute into the GC or solute can be extracted from the cartridge with solvent in order to inject into the GC. | |
| Packed column [56] | Similar to the inert gas stripping method. Column just has packing in it. | Packing eliminates problem of aerosols/bursting bubbles at surface |
| Counterflow packed column[56, 57] | Water-saturated air flows up through a packed column. The test solution flows down through the column. The exiting solution is collected and analyzed for concentration. | This can be used for compounds with low to moderate volatilities. Recommended range is $1 \cdot 10^{-4} \leq k_H$ (unitless molar concentration basis) $\leq 5 \cdot 10^{-2}$. The stripping factor must be less than 1. If the stripping factor is too small, it can be difficult to measure differences between inlet and outlet concentration. |
| Concurrent flow or wetted wall column [58, 59] | Solute-saturated water enters the wetted-wall column where it is in contact with a concurrent flow of gas (air). The two streams are separated at the bottom of the column and analyzed using GC. | The system must be validated to ensure full equilibrium is reached within the column [27]. |
| Horizontal Flow Reactor [60] | This method is a cross between the wetted wall column method and evaporation from a water surface. $N_2$ is blown through a horiztonal tube. A container of water is sitting stagnant on the bottom of the tube. | |
| Evaporation from a water surface [61] | Air is blown across the top of a solution at a known flow rate to evaporate the solute. The concentrations of solute in the water and gas phases are measured. Equilibrium is not achieved, so estimated mass transfer coefficients are used to determine the departure from equilibrium. | This method is for substances with low air-water partition coefficients that aggregate in solution, ionize, or display surface activity. Recommended range is $k_H$ (unitless molar concentration basis) $< 10^{-3}$. |
| Diffusion in air and water boundary layers [62] | $k_H$ is obtained from two partition coefficients between polydimetholsiloxane (PDMS) and air and between PDMS and water. Partition coefficients with PDMS are determined by measuring the mass transfer rate constants in the boundary layer. | |

Table A.3: $\gamma_i^\infty$ experimental methods

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| VLE extrapolation [63] | VLE data can be fit using a Gibbs excess model (i.e. Margules, Wilson, NRTL, etc.) which will give activity coefficients as a function of composition, and $\gamma_i^\infty$s are obtained from these models by extrapolating to infinite dilution [43, 63] | This assumes that extrapolating is valid. |
| Relative GLC (RGLC) [63, 64] | This uses an internal standard during measurement, so one $\gamma_i^\infty$ of a solute must be known for each solvent. Two solutes are run through the GC simultaneously. The ratio of $\gamma_i^\infty$s is determined by measurement of the retention times of the components. | This method is applicable to a wide range of solvent volatilities[40]. The solute must be more volatile than solvent. One reference states this method can have a precision of ≥ 5% [64]. Errors that go into the calculation include vapor pressure errors and the error of the reference value. |
| Isopiestic Method [23] | The partial pressure of water is controlled using calcium chloride solutions (or another drying agent). Equilibrium with the organic-rich phase is obtained through the vapor phase. $\gamma_i^\infty$ is determined from measurement of water in the organic phase. | |
| Non-Steady-State Gas-Liquid Chromatography (NSGC) [63] or NSGLC | A slug of liquid solvent with an appreciable vapor pressure is injected into the GC column. The solvent condenses on the solid support and then equilibrates with the carrier gas. The solvent then bleeds out of the column at a steady rate. Solute is repeatedly injected over a period of time. The retention times of the solute will decrease at the same rate as the rate of the solvent evaporation. The retention times are related to a retention differential parameter which is used to determine $\gamma_i^\infty$. | The exact amount of the stationary phase or solvent does not need to be known, so it avoids the greatest source of error for measurement of $\gamma_i^\infty$ with volatile solvents. Effects of adsorption probably cancel out due to the use of retention differences [43]. It is only applicable for systems in which the solute is more volatile than the solvent, and it cannot be used to study mixed solvents. This method is considered less accurate than others [40]. If a compressibility correction is used, the accuracy can get to 3 %. A practical upper bound may be a relative volatility of 100. The applicability for water as the solvent is the range 23–350 K. |
| Gas-Liquid Chromatography (GLC) [63, 65] | A column is prepared with a solvent supported on an inert solid. An inert carrier gas is passed through the column, and the retention behavior of the solute is measured. Some authors include a gas phase correction. | This method does not work as well with volatile solvents [63, 66]. The major source of error in this method is the weight of solvent in the column because it is difficult to determine accurately. Some researchers claim precisions of 1-3% are possible [40, 43]. Adsorption problems have been noted for aqueous systems [48]. Solvent purity is critical in this method, but solute purity is not due to separation in the chromatograph [65]. This is one of the fastest methods. A recommended range is 0.0005 < $k_H$ (unitless molar concentration basis) < 0.05. |

Table A.3: $\gamma_i^\infty$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Headspace GLC (HGLC) [40, 48, 67] | The headspace above a solution is analyzed using GC and the response is related to $\gamma_i^\infty$. | The major limitation is the lack of high quality experimental gas phase virial coefficients needed to correct for pressure. A recommended range is $20 < k_H$ (unitless molar concentration basis) $< 20{,}000$. For insoluble solutes or low $k_H$s, the RGLC or gas stripping methods are preferred. Under good conditions, HGLC can give precision within 1-5%. |
| Indirect HGLC [68] | Indirect HGLC measures the hexadecane-water partition coefficient and relates it to $\gamma_i^\infty$. The solute GC peak area of the vapor phase in equilibrium with a dilute aqueous solution is measured, and then it is measured again after the addition of a known volume of hexadecane. The partition coefficient is determined from the ratio of GC peak areas and the volume of hexadecane which is then related to $\gamma_i^\infty$. | This method does not require a standard solution of the solute or calibration of the detector. However, it does require that the air-hexadecane partition coefficient be known. The solute must be volatile enough to be detected in the headspace of the water-hexadecane system. |
| Liquid-Liquid Chromatography (LLC) [66] | LLC is used to determine the $\gamma_i^\infty$ ratio of a solute between a mobile and stationary phase which is a liquid on a solid support. It is necessary to determine $\gamma_i^\infty$ of the solute in one of the phases using another technique in order to determine $\gamma_i^\infty$ in the other phase. | This method is only accurate if the mutual solubilities of the stationary phase and mobile phase are negligible. The accuracy of this method is not as high as the GC techniques [43]. There have been reported adsorption problems for aqueous systems [48]. |
| Gas stripping | See description in Table A.2. | |
| EXPSAT method [40] | Exponential saturator method. See description in Table A.2. | |
| Differential distillation [40] or transpiration method | A small amount of solute is distilled off (using an inert gas) of a dilution solution so that its composition is essentially unchanged. Concentrations of samples in the distillate and batch solution are determined. | This is recommended for relative volatilites << 1. Relatively large batches of solution are required, so this is a good method for water and inexpensive solvents. |
| Differential Ebulliometry [69] | Differential ebulliometry consists of measuring the difference in boiling points of a pure solvent and the solvent with dissolved solute [70]. The data can be related back to the $\gamma_i^\infty$ through thermodynamics. | Steady state can be achieved fairly quickly [71]; however, steady state may not represent true equilibrium. This method requires characterization of the ebulliometer and accurate determination of the vaporization ratio. Ebulliometry yields accurate results for systems where the limiting relative volatility is near unity [43, 46]. Another recommended range is for relative volatilities between 0.3-20 [48]. The accuracy is not as good for high-boiling-point systems and highly viscous systems [43]. |

## Table A.3: $\gamma_i^\infty$ experimental methods (cont.)

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Rayleigh distillation method [40, 46] (similar to differential distillation) | It is based on a single stage distillation. A dilute solution is prepared in a glass equilibrium cell. An inert gas is introduced into the solution at a flow rate that will ensure complete saturation. When enough solution has been distilled off, the cell is weighed, and the solution is analyzed using chromatography. The GC peak response and mass ratios are related to $\gamma_i^\infty$. | Dilute solutions must be used. This method can reach precision of 1%. A flow rate of about 0.2 $cm^3/s$ is required for aqueous solutions. A recommended range for relative volatilities is 1-70. |
| Differential static cell method [43, 72] | The differences in equilibrium vapor pressure are measured at constant temperature between a dilute solution and the pure solvent as a function of composition in the dilute solution. For solutes with similar volatility as water, liquid composition is determined gravimetrically. Since composition is not measured directly, a vaporization correction must be made for volatile solutes since they vaporize into the headspace. | This method has been applied to measure solubility without a compositional analysis. A correction must be made to measured data, but this method is better than others (such as ebulliometry) for solvents with poor boiling properties (such as water or polymer solutions) or for mixtures with high relative volatility. |
| Circulation Still [40, 73] | VLE circulation still operated at constant pressure used to provide samples of corresponding vapor and liquid compositions. No measurement of temperature needed as the boiling temp of the solution is indistinguishable from that of the neat solvent. | Recommended ranges are 30 K below the normal boiling temperature of the solvent and a relative volatility between 0.1-30. An uncertainty of 3-5% is possible. |
| Dew-point method [43, 72, 74] | The dew point method is similar to the ebulliometric method. The change in dew temperature of the vapor of a solvent is measured as a small amount of solute is added. | This method works well for systems with relative volatilities below about 0.3. GLC, GS, HGLC, ebulliometry, and the differential static methods all have difficulties measuring $\gamma_i^\infty$ at volatilities this low. This method is typically limited to binary systems of low volatility. |
| Molecular Beams [75] | The vapors from each of two vapor-liquid equilibrium cells are collimated into molecular beams. The beams are alternately chopped before being detected by a mass spectrometer. The output signal from the mass spectrometer will be representative of the difference in partial pressure for any component in the two cells. Differences in pressure between apure component and that containing a species at infinite dilution can be easily detected. | |

## Table A.4: KOW experimental methods

| Experiment | Description | Assumptions/Limits |
|---|---|---|
| Shake flask method [45, 76, 77] | Solute is added to a flask with octanol/water and shaken. The concentrations are determined in the phases using an analytical method. | The recommend range is approximately -2 ≥ logKOW ≥ 4. This method should typically not be used for polycyclic aromatic substances without polar substituents; halogenated hydrocarbons; or large, non-polar chemicals. |
| Generator column [78] | A generator column is packed with a support that is coated in the test chemical at a fixed n-octanol concentration. The solute is eluted from the column with water. The extractor column extracts solute from the aqueous phase, and it is then eluted and analyzed using HPLC or GC. | This can be used for 1 < logKOW < 6. |
| Slow stir method [45, 79] | This method is similar to the shake flask method. The main difference is that the octanol and water phases are slowly stirred instead of shaken while the system reaches equilibrium. | This method prevents the formation of emulsions. It can be used for 5 < logKOW < 8.2. |
| HPLC correlation (indirect) [3, 80, 81] | Chemicals injected into an HPLC column have various retention times. Reference values are used to develop a relationship between the property ($x_i^{aq}$ or KOW) and retention time. This equation is used to find the property of other compounds based on retention time. | Reference substances are needed, so this is sometimes considered an estimation method. Recommended ranges are 0 < logKOW < 6 according to OPPTS and OECD and 0 < logKOW < 8 according to ASTM. This method should not be used for strong acids and bases, metal complexes, or compounds that react with either the eluent or column packing. |

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# Appendix B. Fugacity Error Propagation

The total error of a function can be determined by taking the partial derivatives of the function with respect to all of the variables. In general terms, $y$ is a function of $a$, $b$, $c$, etc.,

$$y = f(a,b,c,...) .$$

The variance in $y$, $s_y$, can be determined using the partial derivatives of the function with respect to all of the variables ($a$, $b$, $c$, etc.) and the variances of the variables ($s_a$, $s_b$, $s_c$, etc.)

$$s_y^2 = \left(\frac{\partial x}{\partial a}\right)^2 s_a^2 + \left(\frac{\partial x}{\partial b}\right)^2 s_b^2 + \left(\frac{\partial x}{\partial c}\right)^2 s_c^2 + \ldots .$$

The error associated with the fugacity ratio,$\Psi$, must be estimated in order to determine the uncertainty of $\gamma_i^\infty$. The natural log of equation 4.15 yields

$$\ln(\Psi_i) = \int_{Tm_i}^{T} \frac{\Delta H_{f,Tm} + \int_{Tm_i}^{T} Cp_i^L \, dT - \int_{Tm_i}^{T} Cp_i^S \, dT}{RT^2} dT .$$

Separating the terms yields:

$$\ln(\Psi_i) = \int_{Tm_i}^{T} \frac{\Delta H_{f,Tm}}{RT^2} dT + \int_{Tm_i}^{T} \frac{\int_{Tm_i}^{T} Cp_i^L \, dT}{RT^2} dT - \int_{Tm_i}^{T} \frac{\int_{Tm_i}^{T} Cp_i^S \, dT}{RT^2} dT .$$

In order to simplify the error estimation, it has been assumed that *Cp*s are constant and that the error in $Tm_i$ is negligible (this was not assumed in the actual calculation). Integrating and combining terms yields:

$$\ln(\Psi_i) = \frac{-\Delta H_{f,Tm}}{R}\left(\frac{1}{T} - \frac{1}{Tm_i}\right) + \frac{Cp_i^L}{R}\left[\ln\left(\frac{T}{Tm_i}\right) + \frac{Tm_i}{T} - 1\right] + \frac{Cp_i^S}{R}\left[-\ln\left(\frac{T}{Tm_i}\right) - \frac{Tm_i}{T} + 1\right].$$

Due to the assumptions made, the error in $\ln(\Psi_i)$ is determined from:

$$s_{\ln\Psi} = \left(\frac{\partial \ln \Psi_i}{\partial \Delta H_{f,Tm}}\right)^2 s_{\Delta Hf,Tm}^2 + \left(\frac{\partial \ln \Psi_i}{\partial Cp_i^L}\right)^2 s_{Cp^L}^2 + \left(\frac{\partial \ln \Psi_i}{\partial Cp_i^S}\right)^2 s_{Cp^S}^2 ,$$

where

$$\frac{\partial \ln \Psi_i}{\partial \Delta H_{f,Tm}} = -\frac{1}{R}\left(\frac{1}{T} - \frac{1}{Tm_i}\right),$$

$$\frac{\partial \ln \Psi_i}{\partial Cp_i^L} = \frac{1}{R}\left[\ln\left(\frac{T}{Tm_i}\right) + \frac{Tm_i}{T} - 1\right],$$

and

$$\frac{\partial \ln \Psi_i}{\partial Cp_i^S} = \frac{1}{R}\left[-\ln\left(\frac{T}{Tm_i}\right) - \frac{Tm_i}{T} + 1\right].$$

The uncertainties for the individual properties were the uncertainties assigned in DIPPR® 801.

# Appendix C. Summary of Recommended Values

The regression coefficients determined in this study are included in this appendix. Coefficients are not included for the API recommendations that were accepted in this study. Abbreviations used throughout the tables are explained in Table C.1.

Table C.1: Abbreviations used in regression tables

| Abbreviation | Explanation |
|---|---|
| D | Data Type |
| E | Experimental |
| EP | Experimental and Predicted |
| P | Predicted |
| S | Smoothed |
| s | Uncertainty of regression |
| Tmin | Minimum temperature of regression (K) |
| Tmax | Maximum temperature of regression (K) |
| U | Unknown |

The compounds within each table are sorted by chemical family. The DIPPR® equation number (Eq) is included for each set of coefficients (see Table 4.3). DIPPR® equation 100 was also used for "regressions" that are only valid at one temperature:

$$Y = A + BT + CT^2 + DT^3 + ET^4 .$$

In these instances, only coefficient "A" was defined.

Table C.2: $k_H$ regression summary

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **1-ALKENES** | | | | | | | | | | | |
| 1-PENTENE | 109-67-1 | 100 | 1.867E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXENE | 592-41-6 | 100 | 2.190E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEPTENE | 592-76-7 | 100 | 2.828E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-OCTENE | 111-66-0 | 100 | 3.555E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-NONENE | 124-11-8 | 100 | 4.854E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-DECENE | 872-05-9 | 100 | 6.459E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-UNDECENE | 872-05-9 | 100 | 8.669E+06 | -1.003E+04 | -3.126E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-DODECENE | 872-05-9 | 100 | 1.108E+07 | -5.042E+04 | -2.173E+02 | 2.501E-01 | 1 | 298.15 | 298.15 | < 25% | P |
| 1-TRIDECENE | 592-41-6 | 100 | 1.513E+07 | -1.203E+04 | -3.844E+01 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-TETRADECENE | 872-05-9 | 100 | 1.827E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-PENTADECENE | 13360-61-7 | 100 | 2.493E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **2,3,4-ALKENES** | | | | | | | | | | | |
| cis-2-PENTENE | 627-20-3 | 100 | 1.262E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| trans-2-PENTENE | 646-04-8 | 100 | 1.293E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| cis-2-HEPTENE | 6443-92-1 | 100 | 2.341E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| trans-2-HEPTENE | 14686-13-6 | 100 | 2.292E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| **ACETATES** | | | | | | | | | | | |
| METHYL ACETATE | 79-20-9 | 101 | 4.579E+02 | -2.509E+04 | -6.446E+01 | 0 | 0 | 293.15 | 343.25 | < 10% | E |
| ETHYL ACETATE | 141-78-6 | 101 | 2.419E+02 | -1.524E+04 | -3.230E+01 | 0 | 0 | 288.15 | 353.15 | < 10% | E |
| n-PROPYL ACETATE | 109-60-4 | 101 | 2.912E+02 | -1.778E+04 | -3.939E+01 | 0 | 0 | 298 | 343.25 | < 10% | E |
| n-BUTYL ACETATE | 123-86-4 | 101 | 2.499E+02 | -1.619E+04 | -3.305E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| ISOBUTYL ACETATE | 110-19-0 | 101 | 8.284E+01 | -8.464E+03 | -8.209E+00 | 0 | 0 | 273.15 | 323.15 | < 25% | E |
| ISOPENTYL ACETATE | 123-92-2 | 101 | 3.240E+02 | -1.974E+04 | -4.386E+01 | 0 | 0 | 273.15 | 363.85 | < 10% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ISOPROPYL ACETATE | 108-21-4 | 101 | -6.279E+01 | -2.050E+03 | 1.353E+01 | 0 | 0 | 273.15 | 310.2 | < 25% | E |
| sec-BUTYL ACETATE | 105-46-4 | 101 | 2.287E+02 | -1.494E+04 | -2.998E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| VINYL ACETATE | 108-05-4 | 101 | 1.816E+02 | -1.163E+04 | -2.364E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |
| n-PENTYL ACETATE | 628-63-7 | 101 | 4.256E+02 | -2.473E+04 | -5.879E+01 | 0 | 0 | 273.15 | 364.5 | < 25% | E |
| n-HEXYL ACETATE | 142-92-7 | 101 | 4.425E+02 | -2.542E+04 | -6.131E+01 | 0 | 0 | 273.15 | 363.35 | < 25% | E |
| n-HEPTYL ACETATE | 112-06-1 | 101 | 3.811E+03 | 1.191E+02 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| n-OCTYL ACETATE | 112-14-1 | 101 | 5.471E+03 | -1.036E+04 | -3.420E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| tert-BUTYL ACETATE | 540-88-5 | 101 | 2.451E+02 | -1.574E+04 | -3.227E+01 | 0 | 0 | 273.15 | 353.65 | < 10% | E |
| CYCLOHEXYL ACETATE | 622-45-7 | 101 | 2.617E+02 | -1.729E+04 | -3.465E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| PHENYL ACETATE | 122-79-2 | 101 | 2.503E+02 | -1.713E+04 | -3.319E+01 | 0 | 0 | 273.15 | 363.95 | < 10% | E |
| **ALDEHYDES** | | | | | | | | | | | |
| ACETALDEHYDE | 75-07-0 | 101 | 2.462E+01 | -5.570E+03 | 0 | 0 | 0 | 273 | 318.15 | < 10% | E |
| PROPANAL | 123-38-6 | 101 | 2.821E+02 | -1.701E+04 | -3.844E+01 | 0 | 0 | 278.15 | 318.15 | < 5% | E |
| BUTANAL | 123-72-8 | 101 | 2.664E+01 | -6.032E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| 2-METHYLPROPANAL | 78-84-2 | 100 | 1.093E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | S |
| PENTANAL | 110-62-3 | 101 | 2.851E+01 | -6.494E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| HEPTANAL | 111-71-7 | 101 | 3.256E+01 | -7.502E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| HEXANAL | 66-25-1 | 101 | 2.848E+01 | -6.372E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| OCTANAL | 124-13-0 | 101 | 3.253E+01 | -7.342E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 10% | E |
| NONANAL | 124-19-6 | 101 | 3.145E+01 | -6.837E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| 2-ETHYLHEXANAL | 123-05-7 | 101 | 2.662E+01 | -5.414E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| 2-ETHYL-2-HEXENAL | 645-62-5 | 101 | 2.647E+01 | -5.815E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 50% | E |
| DECANAL | 112-31-2 | 101 | 3.897E+01 | -8.912E+03 | 0 | 0 | 0 | 298.15 | 318.15 | < 50% | E |
| 2-METHYL-BUTYRALDEHYDE | 96-17-3 | 101 | 2.641E+01 | -5.574E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | P |
| ACROLEIN | 107-02-8 | 101 | 2.385E+01 | -5.131E+03 | 0 | 0 | 0 | 273 | 298 | < 100% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| trans-CROTONALDEHYDE | 123-73-9 | 101 | 1.928E+02 | -1.287E+04 | -2.545E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | EP |
| METHACROLEIN | 78-85-3 | 101 | 2.256E+01 | -4.605E+03 | 0 | 0 | 0 | 273.15 | 333.15 | < 10% | E |
| p-TOLUALDEHYDE | 104-87-0 | 101 | 2.876E+01 | -7.189E+03 | 0 | 0 | 0 | 278 | 298 | < 25% | E |
| BENZALDEHYDE | 100-52-7 | 101 | 5.844E+02 | -3.018E+04 | -8.394E+01 | 0 | 0 | 273.08 | 323.15 | < 10% | E |
| m-TOLUALDEHYDE | 620-23-5 | 101 | 2.911E+01 | -7.166E+03 | 0 | 0 | 0 | 278 | 298 | < 25% | E |
| **ALIPHATIC ETHERS** | | | | | | | | | | | |
| DIETHYL ETHER | 60-29-7 | 101 | 2.854E+02 | -1.727E+04 | -3.841E+01 | 0 | 0 | 273.35 | 333.25 | < 5% | E |
| DIISOPROPYL ETHER | 108-20-3 | 101 | -1.401E+01 | -4.538E+03 | 6.784E+00 | 0 | 0 | 273.15 | 334.15 | < 10% | E |
| DI-n-BUTYL ETHER | 142-96-1 | 101 | 3.269E+01 | -6.711E+03 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| METHYL tert-BUTYL ETHER | 1634-04-4 | 101 | 1.038E+02 | -9.286E+03 | -1.129E+01 | 0 | 0 | 273.15 | 343.15 | < 10% | E |
| METHYL ISOBUTYL ETHER | 625-44-5 | 101 | 3.182E+01 | -6.669E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 5% | E |
| DI-n-HEXYL ETHER | 112-58-3 | 101 | 8.915E+04 | -7.488E+03 | -2.548E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| METHYL n-BUTYL ETHER | 628-28-4 | 101 | 7.536E+02 | -3.836E+04 | -1.081E+02 | 0 | 0 | 273.15 | 298.15 | < 25% | E |
| DI-n-PENTYL ETHER | 693-65-2 | 101 | 5.151E+04 | -5.574E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| METHYL tert-PENTYL ETHER | 994-05-8 | 101 | 2.294E+02 | -1.545E+04 | -2.965E+01 | 0 | 0 | 273.15 | 352.35 | < 10% | E |
| tert-BUTYL ETHYL ETHER | 637-92-3 | 101 | 3.193E+01 | -6.851E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| ETHYL tert-PENTYL ETHER | 919-94-8 | 101 | 3.404E+01 | -7.373E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| DI-n-PROPYL ETHER | 111-43-3 | 101 | 4.575E+02 | -2.541E+04 | -6.361E+01 | 0 | 0 | 273.15 | 333.25 | < 5% | E |
| n-BUTYL ETHYL ETHER | 628-81-9 | 101 | 2.585E+02 | -1.600E+04 | -3.439E+01 | 0 | 0 | 273.15 | 363.85 | < 25% | E |
| **ALKYLCYCLOHEXANES** | | | | | | | | | | | |
| METHYLCYCLOHEXANE | 108-87-2 | 101 | 4.101E+02 | -2.147E+04 | -5.678E+01 | 0 | 0 | 293.15 | 443.95 | < 25% | E |
| ETHYLCYCLOHEXANE | 1678-91-7 | 101 | 1.847E+03 | -6.190E+04 | -3.046E+02 | 3.719E-01 | 1 | 273.15 | 443.95 | < 10% | E |
| cis-1,2-DIMETHYLCYCLOHEXANE | 2207-01-4 | 101 | 3.907E+02 | -2.062E+04 | -5.388E+01 | 0 | 0 | 273.15 | 313.15 | < 25% | E |
| trans-1,2-DIMETHYL- | 6876-23-9 | 101 | 1.558E+03 | -5.359E+04 | -2.548E+02 | 2.970E-01 | 1 | 273.15 | 443.25 | < 5% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CYCLOHEXANE | | | | | | | | | | | |
| **ALKYLCYCLOPENTANES** | | | | | | | | | | | |
| METHYL-CYCLOPENTANE | 96-37-7 | 100 | 2.005E+06 | 7.831E+03 | 2.727E+01 | 6.321E-06 | 2 | 298.15 | 298.15 | < 3% | S |
| **ALKYNES** | | | | | | | | | | | |
| ETHYLACETYLENE | 107-00-6 | 100 | 9.853E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-PENTYNE | 627-19-0 | 100 | 1.436E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXYNE | 693-02-7 | 100 | 2.093E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-OCTYNE | 629-05-0 | 100 | 4.445E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-NONYNE | 3452-09-3 | 100 | 6.477E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEPTYNE | 628-71-7 | 100 | 3.050E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **AROMATIC ALCOHOLS** | | | | | | | | | | | |
| 2,3-XYLENOL | 526-75-0 | 101 | 2.249E+01 | -6.077E+03 | 0 | 0 | 0 | 349.05 | 371.65 | < 25% | S |
| 2,4-XYLENOL | 105-67-9 | 101 | 2.115E+01 | -5.479E+03 | 0 | 0 | 0 | 349.05 | 371.65 | < 25% | E |
| 2,5-XYLENOL | 95-87-4 | 101 | 4.433E+02 | -2.706E+04 | -6.154E+01 | 0 | 0 | 278 | 371.65 | < 10% | E |
| 2,6-XYLENOL | 576-26-1 | 101 | 1.892E+02 | -1.364E+04 | -2.455E+01 | 0 | 0 | 278 | 371.65 | < 10% | E |
| 3,4-XYLENOL | 95-65-8 | 101 | 2.495E+01 | -7.210E+03 | 0 | 0 | 0 | 293.15 | 371.65 | < 25% | E |
| 3,5-XYLENOL | 108-68-9 | 101 | 1.997E+02 | -1.533E+04 | -2.580E+01 | 0 | 0 | 293.15 | 371.65 | < 25% | E |
| PHENOL | 108-95-2 | 101 | 5.283E+02 | -3.105E+04 | -7.428E+01 | 0 | 0 | 278 | 373.15 | < 25% | E |
| o-CRESOL | 95-48-7 | 101 | 3.028E+02 | -1.968E+04 | -4.119E+01 | 0 | 0 | 293.15 | 371.65 | < 5% | E |
| m-CRESOL | 108-39-4 | 101 | 7.124E+01 | -8.354E+03 | -7.310E+00 | 0 | 0 | 298.15 | 371.65 | < 25% | E |
| p-CRESOL | 106-44-5 | 101 | 1.167E+02 | -1.074E+04 | -1.390E+01 | 0 | 0 | 298 | 371.65 | < 3% | E |
| 2-PHENYLETHANOL | 60-12-8 | 101 | 2.325E+02 | -1.641E+04 | -3.094E+01 | 0 | 0 | 283.15 | 373.15 | < 10% | P |
| **AROMATIC AMINES** | | | | | | | | | | | |
| o-TOLUIDINE | 95-53-4 | 101 | 2.612E+01 | -7.057E+03 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |
| m-TOLUIDINE | 108-44-1 | 101 | 2.644E+01 | -7.202E+03 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |
| p-TOLUIDINE | 106-49-0 | 101 | 1.765E+01 | -4.381E+03 | 0 | 0 | 0 | 293.15 | 313.15 | < 5% | P |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| N,N-DIETHYLANILINE | 91-66-7 | 101 | 2.913E+01 | -6.682E+03 | 0 | 0 | 0 | 273.15 | 333.15 | < 25% | E |
| PYRIDINE | 110-86-1 | 101 | 1.987E+01 | -4.699E+03 | 0 | 0 | 0 | 298 | 374.15 | < 25% | E |
| ANILINE | 62-53-3 | 101 | 2.395E+02 | -1.634E+04 | -3.199E+01 | 0 | 0 | 298 | 374.15 | < 10% | E |
| 2-METHYLPYRIDINE | 109-06-8 | 101 | 2.533E+01 | -6.348E+03 | 0 | 0 | 0 | 298 | 313.15 | < 5% | E |
| o-ETHYLANILINE | 578-54-1 | 101 | 2.240E+02 | -1.605E+04 | -2.933E+01 | 0 | 0 | 283.15 | 363.15 | < 10% | P |
| DIBENZOPYRROLE | 86-74-8 | 101 | 1.387E+01 | -4.292E+03 | 0 | 0 | 0 | 278.15 | 308.15 | < 50% | E |
| 2,6-DIMETHYL-PYRIDINE | 108-48-5 | 101 | 2.870E+01 | -7.334E+03 | 0 | 0 | 0 | 298 | 313.15 | < 25% | E |
| 3-METHYLPYRIDINE | 108-99-6 | 101 | 2.516E+01 | -6.371E+03 | 0 | 0 | 0 | 298 | 313.15 | < 25% | E |
| 4-METHYLPYRIDINE | 108-89-4 | 101 | 2.527E+01 | -6.484E+03 | 0 | 0 | 0 | 298 | 313.15 | < 5% | E |
| 2,4-DIMETHYLANILINE | 95-68-1 | 101 | 3.271E+02 | -2.102E+04 | -4.451E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | P |
| N-ETHYLANILINE | 103-69-5 | 101 | 2.866E+02 | -1.928E+04 | -3.821E+01 | 0 | 0 | 273.15 | 363.15 | < 10% | E |
| **AROMATIC CHLORIDES** | | | | | | | | | | | |
| BENZYL CHLORIDE | 100-44-7 | 101 | 2.274E+01 | -4.447E+03 | 0 | 0 | 0 | 277.65 | 303.15 | < 25% | E |
| MONOCHLOROBENZENE | 108-90-7 | 101 | 3.469E+02 | -1.808E+04 | -4.849E+01 | 0 | 0 | 274.15 | 353.16 | < 10% | E |
| o-DICHLOROBENZENE | 95-50-1 | 101 | 8.041E+02 | -3.979E+04 | -1.161E+02 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| m-DICHLOROBENZENE | 541-73-1 | 101 | 2.467E+01 | -4.435E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| p-DICHLOROBENZENE | 106-46-7 | 101 | 5.888E+02 | -3.085E+04 | -8.350E+01 | 0 | 0 | 278.15 | 346.55 | < 10% | E |
| HEXACHLOROBENZENE | 118-74-1 | 101 | 3.108E+01 | -6.570E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| o-CHLOROTOLUENE | 95-49-8 | 101 | 2.530E+01 | -4.528E+03 | 0 | 0 | 0 | 274.15 | 318.15 | < 25% | E |
| p-CHLOROTOLUENE | 106-43-4 | 101 | 2.621E+01 | -4.854E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 2,4-DICHLOROTOLUENE | 95-73-8 | 101 | 2.660E+01 | -4.973E+03 | 0 | 0 | 0 | 278.15 | 323.1 | < 10% | E |
| 1,2,4-TRICHLOROBENZENE | 120-82-1 | 101 | 3.085E+01 | -6.372E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 1,2,3-TRICHLOROBENZENE | 87-61-6 | 101 | 2.446E+01 | -4.581E+03 | 0 | 0 | 0 | 277.15 | 323.15 | < 25% | E |
| **AROMATIC ESTERS** | | | | | | | | | | | |
| BENZYL ACETATE | 140-11-4 | 101 | 2.710E+01 | -6.836E+03 | 0 | 0 | 0 | 273.15 | 322.95 | < 25% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DI-n-PROPYL PHTHALATE | 131-16-8 | 100 | 2.556E+00 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DI-n-HEXYL PHTHALATE | 84-75-3 | 100 | 6.687E+00 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| METHYL BENZOATE | 93-58-3 | 101 | 2.728E+02 | -1.738E+04 | -3.673E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ETHYL BENZOATE | 93-89-0 | 101 | 1.896E+02 | -1.354E+04 | -2.429E+01 | 0 | 0 | 273.15 | 363.45 | < 25% | E |
| BENZYL FORMATE | 104-57-4 | 101 | 2.700E+01 | -7.056E+03 | 0 | 0 | 0 | 273.15 | 322.85 | < 25% | E |
| DIETHYL PHTHALATE | 84-66-2 | 101 | 3.994E+02 | -2.656E+04 | -5.448E+01 | 0 | 0 | 278.15 | 374.15 | < 10% | E |
| DI-n-BUTYL PHTHALATE | 84-74-2 | 101 | 9.165E+02 | -5.076E+04 | -1.307E+02 | 0 | 0 | 283.15 | 323.15 | < 25% | E |
| DIMETHYL PHTHALATE | 131-11-3 | 101 | 2.739E+02 | -1.899E+04 | -3.688E+01 | 0 | 0 | 283.15 | 374.15 | < 10% | EP |
| **C, H, BR COMPOUNDS** | | | | | | | | | | | |
| BROMOMETHANE | 74-83-9 | 101 | 2.316E+01 | -3.762E+03 | 0 | 0 | 0 | 273.15 | 305.15 | < 25% | E |
| BROMOETHANE | 74-96-4 | 101 | 2.373E+01 | -3.906E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 3% | E |
| 1,1,2,2-TETRABROMOETHANE | 79-27-6 | 101 | 1.252E+01 | -1.268E+03 | 0 | 0 | 0 | 298.15 | 323.15 | < 50% | E |
| 1-BROMOPROPANE | 106-94-5 | 101 | 2.624E+01 | -4.582E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| 2-BROMOPROPANE | 75-26-3 | 101 | 3.871E+02 | -2.007E+04 | -5.419E+01 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| 1-BROMOBUTANE | 109-65-9 | 100 | 7.447E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-BROMOHEPTANE | 629-04-9 | 100 | 2.483E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1,2-DIBROMOETHANE | 106-93-4 | 101 | 2.246E+01 | -4.218E+03 | 0 | 0 | 0 | 273.15 | 363.75 | < 10% | E |
| m-DIBROMOBENZENE | 108-36-1 | 100 | 4.750E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| BROMOBENZENE | 108-86-1 | 101 | 4.526E+02 | -2.357E+04 | -6.390E+01 | 0 | 0 | 283.15 | 343.15 | < 10% | E |
| TRIBROMOMETHANE | 75-25-2 | 101 | 2.420E+01 | -4.824E+03 | 0 | 0 | 0 | 283 | 313.15 | < 10% | E |
| DIBROMOMETHANE | 74-95-3 | 101 | 1.239E+02 | -8.812E+03 | -1.508E+01 | 0 | 0 | 273.15 | 363.25 | < 5% | E |
| 2-BROMOBUTANE | 78-76-2 | 100 | 6.319E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| p-BROMOTOLUENE | 106-38-7 | 101 | 2.572E+01 | -4.794E+03 | 0 | 0 | 0 | 293.1 | 322.91 | < 25% | E |
| **C, H, F COMPOUNDS** | | | | | | | | | | | |
| METHYL FLUORIDE | 593-53-3 | 101 | 1.396E+02 | -7.560E+03 | -1.805E+01 | 0 | 0 | 273.21 | 353.4 | < 3% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PERFLUORO-n-HEXANE | 355-42-0 | 100 | 5.966E+09 | 1.272E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-OCTANE | 307-34-6 | 100 | 6.880E+10 | -2.945E+04 | -9.548E+01 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| 1,2-DIFLUOROBENZENE | 367-11-3 | 101 | 2.309E+01 | -3.710E+03 | 0 | 0 | 0 | 298.15 | 322.89 | < 25% | E |
| FLUOROBENZENE | 462-06-6 | 101 | 1.836E+02 | -1.116E+04 | -2.381E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | E |
| HEXAFLUOROBENZENE | 392-56-3 | 101 | 3.285E+02 | -1.839E+04 | -4.470E+01 | 0 | 0 | 281.46 | 339.76 | < 3% | E |
| PERFLUORO-n-PENTANE | 678-26-2 | 100 | 1.211E+09 | 5.338E+02 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-HEPTANE | 335-57-9 | 100 | 1.828E+10 | -4.822E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| **C, H, I COMPOUNDS** | | | | | | | | | | | |
| METHYL IODIDE | 74-88-4 | 101 | 3.635E+02 | -1.838E+04 | -5.118E+01 | 0 | 0 | 273.15 | 322.91 | < 5% | E |
| ETHYL IODIDE | 75-03-6 | 101 | 3.349E+02 | -1.753E+04 | -4.661E+01 | 0 | 0 | 273.15 | 303.15 | < 3% | E |
| n-PROPYL IODIDE | 107-08-4 | 101 | 2.604E+01 | -4.523E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| ISOPROPYL IODIDE | 75-30-9 | 101 | 2.673E+01 | -4.664E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| IODOBENZENE | 591-50-4 | 101 | 1.569E+00 | 2.185E+03 | 0 | 0 | 0 | 298 | 303.15 | < 25% | E |
| n-HEXYL IODIDE | 638-45-9 | 100 | 1.635E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| n-BUTYL IODIDE | 542-69-8 | 100 | 8.057E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **C, H, MULTIHALOGEN COMPOUNDS** | | | | | | | | | | | |
| DICHLORODIFLUORO-METHANE | 75-71-8 | 101 | 2.848E+02 | -1.478E+04 | -3.876E+01 | 0 | 0 | 274 | 313.9 | < 25% | E |
| TRICHLOROFLUORO-METHANE | 75-69-4 | 101 | 2.471E+01 | -3.438E+03 | 0 | 0 | 0 | 274 | 313.9 | < 10% | E |
| 1,1,2-TRICHLOROTRIFLUORO-ETHANE | 76-13-1 | 101 | 2.823E+01 | -4.110E+03 | 0 | 0 | 0 | 275.15 | 303.15 | < 25% | E |
| **C, H, NO2 COMPOUNDS** | | | | | | | | | | | |
| NITROMETHANE | 75-52-5 | 101 | 2.448E+02 | -1.397E+04 | -3.386E+01 | 0 | 0 | 273.15 | 363.15 | < 10% | E |
| NITROETHANE | 79-24-3 | 101 | 1.804E+02 | -1.174E+04 | -2.377E+01 | 0 | 0 | 273.15 | 363.25 | < 5% | E |
| 1-NITROPROPANE | 108-03-2 | 101 | 2.032E+02 | -1.313E+04 | -2.688E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| 2-NITROPROPANE | 79-46-9 | 101 | 1.697E+02 | -1.138E+04 | -2.195E+01 | 0 | 0 | 292.85 | 363.35 | < 3% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-NITROBUTANE | 627-05-4 | 100 | 7.245E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| o-NITROTOLUENE | 88-72-2 | 101 | 2.493E+01 | -5.806E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| p-NITROTOLUENE | 99-99-0 | 101 | 2.804E+01 | -7.129E+03 | 0 | 0 | 0 | 281 | 338 | < 10% | E |
| m-NITROTOLUENE | 99-08-1 | 101 | 2.866E+01 | -6.962E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 25% | E |
| NITROBENZENE | 98-95-3 | 101 | 2.229E+02 | -1.487E+04 | -2.953E+01 | 0 | 0 | 283.15 | 372.85 | < 5% | E |
| 2,4-DINITROTOLUENE | 121-14-2 | 101 | 2.605E+02 | -1.830E+04 | -3.489E+01 | 0 | 0 | 277.15 | 334.95 | < 5% | E |
| 2,6-DINITROTOLUENE | 606-20-2 | 101 | 2.793E+01 | -7.598E+03 | 0 | 0 | 0 | 278 | 314 | < 5% | E |
| 3,4-DINITROTOLUENE | 610-39-9 | 101 | 3.267E+01 | -9.586E+03 | 0 | 0 | 0 | 278.2 | 313.2 | < 5% | E |
| 2,4,6-TRINITROTOLUENE | 118-96-7 | 101 | 1.351E+02 | -1.270E+04 | -1.661E+01 | 0 | 0 | 275.55 | 334.15 | < 10% | E |
| **C1/C2 ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| CARBON TETRACHLORIDE | 56-23-5 | 101 | 3.746E+02 | -1.968E+04 | -5.206E+01 | 0 | 0 | 273.15 | 366.15 | < 5% | E |
| METHYL CHLORIDE | 74-87-3 | 101 | 1.775E+02 | -9.830E+03 | -2.345E+01 | 0 | 0 | 273.15 | 366.15 | < 10% | E |
| ETHYL CHLORIDE | 75-00-3 | 101 | 1.936E+02 | -1.056E+04 | -2.581E+01 | 0 | 0 | 281.15 | 366.15 | < 25% | E |
| VINYL CHLORIDE | 75-01-4 | 101 | 3.305E+01 | -3.487E+03 | -1.681E+00 | 0 | 0 | 273.35 | 366.15 | < 25% | E |
| DICHLOROMETHANE | 75-09-2 | 101 | 1.263E+02 | -7.983E+03 | -1.578E+01 | 0 | 0 | 273.15 | 366.15 | < 10% | E |
| CHLOROFORM | 67-66-3 | 101 | 2.287E+02 | -1.327E+04 | -3.056E+01 | 0 | 0 | 273.15 | 366.15 | < 3% | E |
| 1,1-DICHLOROETHANE | 75-34-3 | 101 | 2.587E+02 | -1.445E+04 | -3.508E+01 | 0 | 0 | 273.15 | 366.15 | < 5% | E |
| 1,2-DICHLOROETHANE | 107-06-2 | 101 | 2.782E+02 | -1.560E+04 | -3.810E+01 | 0 | 0 | 273.15 | 366.15 | < 10% | E |
| 1,1,2-TRICHLOROETHANE | 79-00-5 | 101 | 1.159E+02 | -8.493E+03 | -1.384E+01 | 0 | 0 | 273.15 | 363.95 | < 5% | E |
| HEXACHLOROETHANE | 67-72-1 | 101 | 3.026E+01 | -6.068E+03 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| 1,1,1-TRICHLOROETHANE | 71-55-6 | 101 | 7.812E+01 | -6.437E+03 | -7.910E+00 | 0 | 0 | 273.15 | 348.15 | < 10% | E |
| 1,1,1,2-TETRACHLOROETHANE | 630-20-6 | 101 | 2.594E+01 | -4.909E+03 | 0 | 0 | 0 | 273.15 | 323.15 | < 10% | E |
| 1,1,2,2-TETRACHLOROETHANE | 79-34-5 | 101 | 2.448E+01 | -4.984E+03 | 0 | 0 | 0 | 283.15 | 328.65 | < 10% | E |
| TRICHLOROETHYLENE | 79-01-6 | 101 | 2.642E+02 | -1.488E+04 | -3.570E+01 | 0 | 0 | 274.22 | 366.15 | < 5% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| TETRACHLOROETHYLENE | 127-18-4 | 101 | 3.077E+02 | -1.717E+04 | -4.188E+01 | 0 | 0 | 273.15 | 364.95 | < 10% | E |
| cis-1,2-DICHLOROETHYLENE | 156-59-2 | 101 | 2.228E+02 | -1.290E+04 | -2.975E+01 | 0 | 0 | 281.15 | 366.15 | < 10% | E |
| trans-1,2-DICHLOROETHYLENE | 156-60-5 | 101 | 2.410E+01 | -3.940E+03 | 0 | 0 | 0 | 283.15 | 323.15 | < 10% | E |
| PENTACHLOROETHANE | 76-01-7 | 101 | 3.521E+01 | -7.667E+03 | 0 | 0 | 0 | 293.15 | 298 | < 25% | E |
| 1,1-DICHLOROETHYLENE | 75-35-4 | 101 | 3.060E+02 | -1.643E+04 | -4.191E+01 | 0 | 0 | 275.15 | 363.65 | < 10% | E |
| **C3 & HIGHER ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| 1,4-DICHLOROBUTANE | 110-56-5 | 101 | 2.001E+01 | -3.599E+03 | 0 | 0 | 0 | 286.65 | 298.05 | < 10% | E |
| 1,5-DICHLOROPENTANE | 628-76-2 | 101 | 2.216E+01 | -4.045E+03 | 0 | 0 | 0 | 274.15 | 295.85 | < 50% | E |
| 1,2-DICHLOROPROPANE | 78-87-5 | 101 | 2.546E+02 | -1.434E+04 | -3.454E+01 | 0 | 0 | 273.15 | 353.35 | < 10% | E |
| ISOPROPYL CHLORIDE | 75-29-6 | 101 | 2.621E+01 | -4.393E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 10% | E |
| 1,2,3-TRICHLOROPROPANE | 96-18-4 | 101 | 1.366E+01 | -1.857E+03 | 0 | 0 | 0 | 275.05 | 318.15 | < 25% | E |
| HEXACHLORO-1,3-BUTADIENE | 87-68-3 | 101 | 2.978E+01 | -5.451E+03 | 0 | 0 | 0 | 275.15 | 298.15 | < 50% | E |
| PROPYL CHLORIDE | 540-54-5 | 101 | 2.625E+01 | -4.489E+03 | 0 | 0 | 0 | 273.15 | 310.15 | < 10% | E |
| n-BUTYL CHLORIDE | 109-69-3 | 101 | 2.644E+01 | -4.455E+03 | 0 | 0 | 0 | 273.35 | 310.15 | < 10% | E |
| sec-BUTYL CHLORIDE | 78-86-4 | 101 | 2.691E+01 | -4.502E+03 | 0 | 0 | 0 | 275.05 | 298.05 | < 10% | E |
| 1-CHLOROPENTANE | 543-59-9 | 101 | 4.078E+02 | -2.100E+04 | -5.714E+01 | 0 | 0 | 275.65 | 310.15 | < 5% | E |
| 1,3-DICHLOROPROPANE | 142-28-9 | 101 | 1.898E+01 | -3.134E+03 | 0 | 0 | 0 | 275.05 | 303.15 | < 25% | E |
| **CYCLOALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| CYCLOHEXANOL | 108-93-0 | 101 | 2.835E+01 | -7.692E+03 | 0 | 0 | 0 | 298 | 333.15 | < 25% | E |
| **CYCLOALKANES** | | | | | | | | | | | |
| CYCLOPENTANE | 287-92-3 | 101 | 2.262E+02 | -1.246E+04 | -2.995E+01 | 0 | 0 | 298 | 426.25 | < 10% | E |
| CYCLOHEXANE | 110-82-7 | 101 | -1.486E+03 | 3.489E+04 | 2.667E+02 | -4.584E-01 | 1 | 274.25 | 424.15 | < 25% | E |
| CYCLOHEPTANE | 291-64-5 | 100 | 8.267E+05 | -3.094E+04 | -7.154E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | P |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CYCLOOCTANE | 292-64-8 | 101 | 1.860E+02 | -1.172E+04 | -2.337E+01 | 0 | 0 | 273.15 | 313.15 | < 10% | E |
| **CYCLOALKENES** | | | | | | | | | | | |
| CYCLOPENTENE | 142-29-0 | 101 | 2.369E+01 | -3.321E+03 | 0 | 0 | 0 | 283.15 | 298.15 | < 50% | E |
| CYCLOHEXENE | 110-83-8 | 101 | 2.423E+01 | -3.602E+03 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| CYCLOHEPTENE | 628-92-2 | 100 | 2.705E+05 | -8.903E+03 | 0 | 1.478E+06 | -2 | 298.15 | 298.15 | < 25% | E |
| CYCLOOCTENE | 931-88-4 | 101 | 1.856E+02 | -1.135E+04 | -2.370E+01 | 0 | 0 | 273.15 | 313.15 | < 5% | E |
| **DIALKENES** | | | | | | | | | | | |
| 1,4-CYCLOHEXADIENE | 628-41-1 | 101 | 2.424E+01 | -4047.17 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| **DIMETHYLALKANES** | | | | | | | | | | | |
| 2,2-DIMETHYLBUTANE | 75-83-2 | 100 | 9.781E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 2,3-DIMETHYLBUTANE | 79-29-8 | 101 | 3.898E+02 | -2.037E+04 | -5.366E+01 | 0 | 0 | 273.15 | 422.65 | < 25% | E |
| 2,4-DIMETHYLPENTANE | 108-08-7 | 100 | 1.937E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| 3,3-DIMETHYLPENTANE | 562-49-2 | 101 | -1.836E+03 | 4.668E+04 | 3.255E+02 | -5.334E-01 | 1 | 298.15 | 423.64 | < 25% | E |
| 2,2-DIMETHYLHEXANE | 590-73-8 | 101 | 6.831E+02 | -3.353E+04 | -9.718E+01 | 0 | 0 | 273.15 | 313.15 | < 5% | E |
| 2,5-DIMETHYLHEXANE | 592-13-2 | 101 | 8.022E+02 | -3.833E+04 | -1.153E+02 | 0 | 0 | 273.15 | 313.15 | < 3% | E |
| **DIPHENYL/POLYAROMATICS** | | | | | | | | | | | |
| BIPHENYL | 92-52-4 | 101 | 6.933E+02 | -3.653E+04 | -9.889E+01 | 0 | 0 | 293.15 | 337.65 | < 10% | E |
| **EPOXIDES** | | | | | | | | | | | |
| 1,4-DIOXANE | 123-91-1 | 101 | 1.235E+02 | -1.032E+04 | -1.500E+01 | 0 | 0 | 273.35 | 374.15 | < 25% | E |
| TETRAHYDROPYRAN | 142-68-7 | 101 | 2.170E+02 | -1.432E+04 | -2.851E+01 | 0 | 0 | 273.35 | 328.15 | < 5% | E |
| TETRAHYDROFURAN | 109-99-9 | 101 | 2.492E+01 | -5.663E+03 | 0 | 0 | 0 | 273.35 | 328.15 | < 10% | E |
| DIBENZOFURAN | 132-64-9 | 101 | 2.617E+01 | -5.831E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| **FORMATES** | | | | | | | | | | | |
| METHYL FORMATE | 107-31-3 | 101 | 1.995E+01 | -3.806E+03 | 0 | 0 | 0 | 285.65 | 333.25 | < 10% | E |
| ETHYL FORMATE | 109-94-4 | 101 | 2.076E+01 | -3.974E+03 | 0 | 0 | 0 | 293.15 | 333.25 | < 25% | E |
| n-PROPYL FORMATE | 110-74-7 | 101 | 2.356E+01 | -4.788E+03 | 0 | 0 | 0 | 272.15 | 333.15 | < 10% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-BUTYL FORMATE | 592-84-7 | 101 | 2.007E+01 | -3.697E+03 | 0 | 0 | 0 | 273.15 | 363.75 | < 25% | E |
| ISOBUTYL FORMATE | 542-55-2 | 101 | 2.564E+01 | -5.223E+03 | 0 | 0 | 0 | 273.15 | 333.55 | < 10% | E |
| n-PENTYL FORMATE | 638-49-3 | 101 | 2.720E+02 | -1.682E+04 | -3.642E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| tert-BUTYL FORMATE | 762-75-4 | 101 | 2.041E+01 | -3.621E+03 | 0 | 0 | 0 | 278.15 | 308.15 | < 5% | E |
| **KETONES** | | | | | | | | | | | |
| ACETONE | 67-64-1 | 101 | 1.327E+02 | -1.016E+04 | -1.639E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| METHYL ETHYL KETONE | 78-93-3 | 101 | 2.253E+02 | -1.451E+04 | -3.000E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 3-PENTANONE | 96-22-0 | 101 | 2.558E+02 | -1.603E+04 | -3.433E+01 | 0 | 0 | 273.15 | 310.2 | < 10% | E |
| METHYL ISOBUTYL KETONE | 108-10-1 | 101 | 2.306E+02 | -1.522E+04 | -3.034E+01 | 0 | 0 | 273.15 | 363.55 | < 10% | E |
| 3-HEPTANONE | 106-35-4 | 101 | 2.236E+02 | -1.559E+04 | -2.890E+01 | 0 | 0 | 273.15 | 363.25 | < 10% | E |
| 4-HEPTANONE | 123-19-3 | 101 | 2.766E+02 | -1.775E+04 | -3.687E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | E |
| 3-HEXANONE | 589-38-8 | 101 | 3.027E+01 | -7.070E+03 | 0 | 0 | 0 | 293.15 | 310.2 | < 10% | E |
| 2-PENTANONE | 107-87-9 | 101 | 2.179E+02 | -1.450E+04 | -2.865E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| METHYL ISOPROPYL KETONE | 563-80-4 | 101 | 2.737E+02 | -1.686E+04 | -3.702E+01 | 0 | 0 | 265.15 | 453.15 | < 10% | P |
| 2-HEXANONE | 591-78-6 | 101 | 1.536E+02 | -1.206E+04 | -1.876E+01 | 0 | 0 | 273.15 | 312.75 | < 10% | E |
| 2-HEPTANONE | 110-43-0 | 101 | 2.878E+02 | -1.827E+04 | -3.858E+01 | 0 | 0 | 273.15 | 363.65 | < 5% | E |
| 5-METHYL-2-HEXANONE | 110-12-3 | 101 | 3.052E+02 | -1.904E+04 | -4.117E+01 | 0 | 0 | 273.15 | 362.85 | < 5% | E |
| 3,3-DIMETHYL-2-BUTANONE | 75-97-8 | 101 | 1.694E+02 | -1.217E+04 | -2.131E+01 | 0 | 0 | 273.15 | 363.35 | < 5% | E |
| DIISOBUTYL KETONE | 108-83-8 | 101 | 3.516E+02 | -2.165E+04 | -4.750E+01 | 0 | 0 | 273.15 | 363.85 | < 10% | E |
| DIISOPROPYL KETONE | 565-80-0 | 101 | 1.603E+02 | -1.197E+04 | -1.972E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| 5-NONANONE | 502-56-7 | 101 | 2.901E+02 | -1.938E+04 | -3.824E+01 | 0 | 0 | 273.15 | 363.75 | < 25% | E |
| 2-NONANONE | 821-55-6 | 101 | 3.154E+02 | -2.001E+04 | -4.227E+01 | 0 | 0 | 273.15 | 364.35 | < 25% | E |
| ACETYLACETONE | 123-54-6 | 101 | 1.685E+01 | -3.780E+03 | 0 | 0 | 0 | 303.15 | 373.15 | < 25% | E |
| CYCLOPENTANONE | 120-92-3 | 101 | 2.341E+01 | -5.848E+03 | 0 | 0 | 0 | 293.2 | 353.15 | < 100% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CYCLOHEXANONE | 108-94-1 | 101 | 2.494E+01 | -6.365E+03 | 0 | 0 | 0 | 298 | 353.15 | < 10% | E |
| 2-OCTANONE | 111-13-7 | 101 | 3.274E+02 | -2.068E+04 | -4.406E+01 | 0 | 0 | 273.15 | 364.15 | < 25% | E |
| ACETOPHENONE | 98-86-2 | 101 | 4.071E+02 | -2.464E+04 | -5.626E+01 | 0 | 0 | 278 | 318.15 | < 25% | E |
| 3-OCTANONE | 106-68-3 | 101 | 1.965E+02 | -1.427E+04 | -2.483E+01 | 0 | 0 | 273.15 | 364.15 | < 10% | E |
| 3-NONANONE | 925-78-0 | 101 | 2.908E+01 | -6.587E+03 | 0 | 0 | 0 | 273.15 | 353.35 | < 25% | E |
| 2,6,8-TRIMETHYL-4-NONANONE | 123-18-2 | 101 | 5.209E+03 | -4.277E+03 | -9.471E+00 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| **MERCAPTANS** | | | | | | | | | | | |
| ISOPROPYL MERCAPTAN | 75-33-2 | 101 | 2.295E+01 | -3.670E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| n-BUTYL MERCAPTAN | 109-79-5 | 101 | 4.008E+02 | -2.101E+04 | -5.613E+01 | 0 | 0 | 288.15 | 333.15 | < 10% | E |
| **METHYLALKANES** | | | | | | | | | | | |
| 2-METHYLPENTANE | 107-83-5 | 101 | 4.013E+02 | -2.096E+04 | -5.529E+01 | 0 | 0 | 273.15 | 422.65 | < 25% | E |
| 3-METHYLPENTANE | 96-14-0 | 100 | 9.326E+06 | 1.259E+04 | 5.099E+01 | -4.402E-02 | 1 | 298.15 | 298.15 | < 3% | S |
| 2-METHYLHEXANE | 591-76-4 | 100 | 1.920E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 3-METHYLHEXANE | 589-34-4 | 100 | 1.716E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 3-METHYLHEPTANE | 589-81-1 | 100 | 2.094E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 4-METHYLHEPTANE | 589-53-7 | 100 | 2.066E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| **METHYLALKENES** | | | | | | | | | | | |
| 2-METHYL-2-BUTENE | 513-35-9 | 101 | 1.486E+02 | -8.954E+03 | -1.839E+01 | 0 | 0 | 273.16 | 322.88 | < 3% | E |
| **N-ALCOHOLS** | | | | | | | | | | | |
| METHANOL | 67-56-1 | 101 | 1.040E+02 | -9.075E+03 | -1.233E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| ETHANOL | 64-17-5 | 101 | 1.745E+02 | -1.301E+04 | -2.237E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-PROPANOL | 71-23-8 | 101 | 2.216E+02 | -1.567E+04 | -2.904E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-BUTANOL | 71-36-3 | 101 | 3.189E+02 | -2.039E+04 | -4.329E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-PENTANOL | 71-41-0 | 101 | 2.743E+02 | -1.835E+04 | -3.661E+01 | 0 | 0 | 273.35 | 371.15 | < 10% | E |
| 1-HEXANOL | 111-27-3 | 101 | 2.987E+02 | -1.978E+04 | -4.003E+01 | 0 | 0 | 298 | 363.15 | < 25% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-HEPTANOL | 111-70-6 | 101 | 3.399E+02 | -2.193E+04 | -4.593E+01 | 0 | 0 | 273 | 375 | < 10% | EP |
| 1-OCTANOL | 111-87-5 | 101 | 4.751E+02 | -2.858E+04 | -6.567E+01 | 0 | 0 | 288.15 | 363.45 | < 10% | EP |
| 1-NONANOL | 143-08-8 | 101 | 4.823E+02 | -2.911E+04 | -6.658E+01 | 0 | 0 | 288.15 | 363.15 | < 25% | E |
| 1-DECANOL | 112-30-1 | 101 | 5.385E+02 | -3.155E+04 | -7.495E+01 | 0 | 0 | 288.15 | 363.15 | < 10% | E |
| 1-UNDECANOL | 112-42-5 | 100 | 4.030E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-DODECANOL | 112-53-8 | 100 | 4.668E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| **N-ALIPHATIC PRIMARY AMINES** | | | | | | | | | | | |
| ETHYLAMINE | 75-04-7 | 100 | 6.618E+01 | 1.162E+04 | 2.974E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-PROPYLAMINE | 107-10-8 | 100 | 8.255E+01 | 1.063E+04 | 2.880E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-BUTYLAMINE | 109-73-9 | 100 | 1.030E+02 | 1.277E+04 | 3.289E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-PENTYLAMINE | 110-58-7 | 100 | 1.284E+02 | 8.883E+03 | 2.125E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-HEXYLAMINE | 111-26-2 | 100 | 1.602E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-HEPTYLAMINE | 111-68-2 | 100 | 1.999E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| n-OCTYLAMINE | 111-86-4 | 100 | 2.493E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **N-ALKANES** | | | | | | | | | | | |
| n-PENTANE | 109-66-0 | 101 | -1.239E+03 | 2.706E+04 | 2.257E+02 | -4.087E-01 | 1 | 273.15 | 422.65 | < 25% | E |
| n-HEXANE | 110-54-3 | 101 | 4.056E+02 | -2.109E+04 | -5.595E+01 | 0 | 0 | 273.15 | 443.15 | < 10% | E |
| n-HEPTANE | 142-82-5 | 101 | 4.213E+02 | -2.189E+04 | -5.819E+01 | 0 | 0 | 273.15 | 443.75 | < 25% | E |
| n-OCTANE | 111-65-9 | 101 | 5.052E+02 | -2.622E+04 | -7.032E+01 | 0 | 0 | 273.15 | 456.15 | < 25% | E |
| n-NONANE | 111-84-2 | 101 | 7.275E+02 | -3.721E+04 | -1.028E+02 | 0 | 0 | 287.95 | 409.75 | < 50% | E |
| n-DECANE | 124-18-5 | 100 | 4.165E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **N-ALKYLBENZENES** | | | | | | | | | | | |
| BENZENE | 71-43-2 | 101 | 6.091E+02 | -2.377E+04 | -9.619E+01 | 9.737E-02 | 1 | 273.15 | 527.15 | < 3% | E |
| TOLUENE | 108-88-3 | 101 | 6.605E+02 | -2.545E+04 | -1.049E+02 | 1.101E-01 | 1 | 261.7 | 473.55 | < 5% | E |
| ETHYLBENZENE | 100-41-4 | 101 | 3.619E+02 | -1.988E+04 | -4.994E+01 | 0 | 0 | 273.15 | 373.15 | < 5% | E |
| n-PROPYLBENZENE | 103-65-1 | 101 | 2.463E+02 | -1.450E+04 | -3.276E+01 | 0 | 0 | 273.65 | 328.15 | < 10% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-BUTYLBENZENE | 104-51-8 | 101 | 4.132E+02 | -2.226E+04 | -5.744E+01 | 0 | 0 | 273.65 | 373.15 | < 5% | E |
| n-HEPTYLBENZENE | 1078-71-3 | 100 | 2.079E+05 | -1.779E+04 | -5.443E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| n-DECYLBENZENE | 104-72-3 | 100 | 7.285E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-PENTYLBENZENE | 538-68-1 | 101 | 4.005E+02 | -2.240E+04 | -5.510E+01 | 0 | 0 | 280.15 | 318.15 | < 10% | E |
| n-HEXYLBENZENE | 1077-16-3 | 101 | 3.675E+02 | -2.136E+04 | -4.985E+01 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| n-OCTYLBENZENE | 2189-60-8 | 100 | 3.005E+05 | 5.570E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| n-NONYLBENZENE | 1081-77-2 | 100 | 3.866E+05 | -4.112E+04 | -2.080E+02 | 2.466E-01 | 1 | 298.15 | 298.15 | < 25% | P |
| **NAPHTHALENES** | | | | | | | | | | | |
| NAPHTHALENE | 91-20-3 | 101 | 3.592E+02 | -2.027E+04 | -4.973E+01 | 0 | 0 | 275.05 | 346.55 | < 3% | E |
| 1-METHYL-NAPHTHALENE | 90-12-0 | 101 | 2.722E+01 | -5.758E+03 | 0 | 0 | 0 | 277.25 | 304.85 | < 10% | E |
| 2-METHYL-NAPHTHALENE | 91-57-6 | 101 | 2.506E+01 | -5.113E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| 1-ETHYL-NAPHTHALENE | 1127-76-0 | 101 | 2.778E+01 | -5.919E+03 | 0 | 0 | 0 | 281.55 | 304.85 | < 10% | E |
| **NITRILES** | | | | | | | | | | | |
| ACETONITRILE | 75-05-8 | 101 | -2.253E+00 | -3.365E+03 | 3.205E+00 | 0 | 0 | 273 | 353.15 | < 5% | E |
| PROPIONITRILE | 107-12-0 | 101 | 9.456E+01 | -7.820E+03 | -1.110E+01 | 0 | 0 | 278.15 | 298.15 | < 25% | E |
| ACRYLONITRILE | 107-13-1 | 101 | 1.926E+01 | -3.863E+03 | 0 | 0 | 0 | 273.15 | 343.15 | < 3% | E |
| METHACRYLONITRILE | 126-98-7 | 101 | 2.729E+02 | -1.537E+04 | -3.756E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | P |
| n-BUTYRONITRILE | 109-74-0 | 101 | 1.333E+02 | -1.001E+04 | -1.650E+01 | 0 | 0 | 273.15 | 313.15 | < 3% | E |
| VALERONITRILE | 110-59-8 | 101 | 2.630E+01 | -6.092E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | E |
| ISOBUTYRONITRILE | 78-82-0 | 101 | 2.382E+01 | -5.246E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | E |
| BENZONITRILE | 100-47-0 | 101 | 3.097E+02 | -1.834E+04 | -4.267E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| VINYLACETONITRILE | 109-75-1 | 101 | 2.209E+01 | -4.916E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| PHENYLACETONITRILE | 140-29-4 | 101 | 2.665E+01 | -6.778E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 100% | E |
| **NITROAMINES** | | | | | | | | | | | |
| o-NITROANILINE | 88-74-4 | 101 | 2.256E+01 | -6.802E+03 | 0 | 0 | 0 | 298.15 | 313.25 | < 50% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| p-NITROANILINE | 100-01-6 | 101 | 2.228E+01 | -8.150E+03 | 0 | 0 | 0 | 293.15 | 313.25 | < 10% | E |
| **ORGANIC SALTS** | | | | | | | | | | | |
| DIETHYL CARBONATE | 105-58-8 | 101 | 3.022E+02 | -1.859E+04 | -4.099E+01 | 0 | 0 | 273.15 | 363.45 | < 5% | E |
| DIMETHYL CARBONATE | 616-38-6 | 101 | 2.193E+02 | -1.373E+04 | -2.937E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |
| **OTHER ALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| ISOPROPANOL | 67-63-0 | 101 | 2.321E+02 | -1.607E+04 | -3.060E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 2-METHYL-1-PROPANOL | 78-83-1 | 101 | 3.840E+02 | -2.321E+04 | -5.299E+01 | 0 | 0 | 273.35 | 374.15 | < 10% | E |
| 2-BUTANOL | 78-92-2 | 101 | 2.945E+02 | -1.939E+04 | -3.956E+01 | 0 | 0 | 273 | 371.15 | < 5% | E |
| 2-METHYL-2-PROPANOL | 75-65-0 | 101 | 2.378E+02 | -1.682E+04 | -3.109E+01 | 0 | 0 | 273 | 371.15 | < 10% | E |
| 2-PENTANOL | 6032-29-7 | 101 | 3.240E+02 | -2.093E+04 | -4.377E+01 | 0 | 0 | 273.35 | 371.15 | < 5% | E |
| 2-METHYL-2-BUTANOL | 75-85-4 | 101 | 2.800E+02 | -1.898E+04 | -3.719E+01 | 0 | 0 | 273.35 | 371.45 | < 5% | E |
| 2-METHYL-1-BUTANOL | 137-32-6 | 101 | 3.671E+02 | -2.288E+04 | -5.021E+01 | 0 | 0 | 273.35 | 363.15 | < 5% | E |
| 2,2-DIMETHYL-1-PROPANOL | 75-84-3 | 101 | 3.360E+02 | -2.136E+04 | -4.548E+01 | 0 | 0 | 285.15 | 363.15 | < 25% | P |
| 2-HEXANOL | 626-93-7 | 101 | 3.326E+02 | -2.148E+04 | -4.486E+01 | 0 | 0 | 273.15 | 363.35 | < 25% | EP |
| 3-HEXANOL | 623-37-0 | 101 | 3.385E+02 | -2.197E+04 | -4.560E+01 | 0 | 0 | 273.15 | 363.45 | < 5% | EP |
| 3-METHYL-1-PENTANOL | 589-35-5 | 101 | 4.097E+02 | -2.540E+04 | -5.620E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | P |
| 3-METHYL-3-PENTANOL | 77-74-7 | 101 | 1.770E+02 | -1.383E+04 | -2.197E+01 | 0 | 0 | 282.95 | 363.55 | < 10% | P |
| 3-PENTANOL | 584-02-1 | 101 | 3.054E+02 | -1.989E+04 | -4.110E+01 | 0 | 0 | 273.35 | 371.15 | < 5% | E |
| 3-METHYL-1-BUTANOL | 123-51-3 | 101 | 4.590E+02 | -2.701E+04 | -6.392E+01 | 0 | 0 | 273.35 | 374.15 | < 10% | E |
| 3-METHYL-2-BUTANOL | 598-75-4 | 101 | 3.121E+02 | -2.017E+04 | -4.208E+01 | 0 | 0 | 273.35 | 371.15 | < 3% | E |
| 2-HEPTANOL | 543-49-7 | 101 | 3.782E+02 | -2.400E+04 | -5.135E+01 | 0 | 0 | 273.15 | 363.35 | < 5% | P |
| 3-HEPTANOL | 589-82-2 | 101 | 3.659E+02 | -2.376E+04 | -4.933E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | E |
| 4-METHYL-2-PENTANOL | 108-11-2 | 101 | 2.657E+02 | -1.777E+04 | -3.520E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | EP |
| 2-OCTANOL | 123-96-6 | 101 | 5.167E+02 | -3.094E+04 | -7.154E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | P |
| 2-NONANOL | 628-99-9 | 101 | 5.400E+02 | -3.288E+04 | -7.444E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | P |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2,6-DIMETHYL-4-HEPTANOL | 108-82-7 | 101 | 2.593E+02 | -1.915E+04 | -3.313E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | P |
| **OTHER ALIPHATIC AMINES** | | | | | | | | | | | |
| DIMETHYLAMINE | 124-40-3 | 100 | 8.902E+01 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| TRIETHYLAMINE | 121-44-8 | 100 | 5.961E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | S |
| DI-n-PROPYLAMINE | 142-84-7 | 100 | 2.576E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DIETHYLAMINE | 109-89-7 | 100 | 1.514E+02 | -1.652E+04 | -4.148E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DI-n-BUTYLAMINE | 111-92-2 | 100 | 4.383E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| TRI-n-BUTYLAMINE | 102-82-9 | 101 | 3.425E+01 | -8.719E+03 | 0 | 0 | 0 | 273.15 | 353.15 | < 25% | E |
| **OTHER ALKANES** | | | | | | | | | | | |
| 2,3,4-TRIMETHYLPENTANE | 565-75-3 | 100 | 1.701E+07 | -1.047E+04 | -3.146E+01 | 0 | 0 | 298.15 | 298.15 | < 5% | P |
| 2,2,5-TRIMETHYLHEXANE | 3522-94-9 | 101 | 3.797E+01 | -6.194E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 10% | E |
| **OTHER ALKYLBENZENES** | | | | | | | | | | | |
| o-XYLENE | 95-47-6 | 101 | 3.284E+02 | -1.815E+04 | -4.516E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | E |
| m-XYLENE | 108-38-3 | 101 | 4.853E+02 | -2.121E+04 | -7.387E+01 | 5.787E-02 | 1 | 273.15 | 543.75 | < 10% | E |
| p-XYLENE | 106-42-3 | 101 | 8.256E+02 | -3.283E+04 | -1.302E+02 | 1.238E-01 | 1 | 273.15 | 568.05 | < 10% | E |
| CUMENE | 98-82-8 | 101 | 2.709E+01 | -4.790E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| 1,2,3-TRIMETHYLBENZENE | 526-73-8 | 101 | 2.534E+01 | -4.560E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| 1,2,4-TRIMETHYLBENZENE | 95-63-6 | 101 | 2.614E+01 | -4.676E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 5% | E |
| MESITYLENE | 108-67-8 | 101 | 2.301E+02 | -1.351E+04 | -3.055E+01 | 0 | 0 | 283.15 | 373.15 | < 25% | E |
| p-DIETHYLBENZENE | 105-05-5 | 101 | 2.841E+04 | 2.844E+03 | 0 | 0 | 0 | 293.15 | 293.15 | < 100% | E |
| 1,2,3,4-TETRAMETHYLBENZENE | 488-23-3 | 101 | 2.968E+01 | -5.913E+03 | 0 | 0 | 0 | 288.15 | 308.15 | < 100% | E |
| 1,2,4,5-TETRAMETHYLBENZENE | 95-93-2 | 100 | 4.079E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| | | | | | | | | | | | |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER AMINES, IMINES** | | | | | | | | | | | |
| CYCLOHEXYLAMINE | 108-91-8 | 101 | 2.024E+02 | -1.528E+04 | -2.596E+01 | 0 | 0 | 298.15 | 372.82 | < 25% | E |
| TRIALLYLAMINE | 102-70-5 | 101 | 4.010E+02 | -2.393E+04 | -5.502E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| **OTHER CONDENSED RINGS** | | | | | | | | | | | |
| FLUORANTHENE | 206-44-0 | 101 | 2.755E+01 | -6.910E+03 | 0 | 0 | 0 | 281.25 | 333.15 | < 10% | E |
| FLUORENE | 86-73-7 | 101 | 2.665E+01 | -6.145E+03 | 0 | 0 | 0 | 279.75 | 333.15 | < 10% | E |
| ANTHRACENE | 120-12-7 | 101 | 3.683E+02 | -2.185E+04 | -5.088E+01 | 0 | 0 | 273.45 | 347.85 | < 5% | E |
| PHENANTHRENE | 85-01-8 | 101 | 4.223E+02 | -2.462E+04 | -5.873E+01 | 0 | 0 | 277.15 | 346.55 | < 5% | E |
| CHRYSENE | 218-01-9 | 101 | 4.104E+01 | -1.184E+04 | 0 | 0 | 0 | 279.65 | 302.15 | < 25% | E |
| PYRENE | 129-00-0 | 101 | 3.078E+02 | -1.937E+04 | -4.193E+01 | 0 | 0 | 277.85 | 347.85 | < 5% | E |
| ACENAPHTHENE | 83-32-9 | 101 | 2.469E+01 | -5.381E+03 | 0 | 0 | 0 | 277.25 | 347.85 | < 25% | E |
| ACENAPHTHALENE | 208-96-8 | 101 | 2.748E+01 | -6.263E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| BENZO[a]PYRENE | 50-32-8 | 101 | 3.108E+01 | -8.515E+03 | 0 | 0 | 0 | 281.15 | 308.15 | < 10% | E |
| BENZO[b]FLUORANTHENE | 205-99-2 | 101 | 1.949E+01 | -5.422E+03 | 0 | 0 | 0 | 283.15 | 328.15 | < 10% | E |
| **OTHER ETHERS/DIETHERS** | | | | | | | | | | | |
| METHYLAL | 109-87-5 | 101 | 2.270E+01 | -4.738E+03 | 0 | 0 | 0 | 273.35 | 333.15 | < 25% | E |
| 1,2-DIMETHOXYETHANE | 110-71-4 | 101 | 2.511E+02 | -1.722E+04 | -3.328E+01 | 0 | 0 | 273.35 | 372.5 | < 3% | E |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 112-73-2 | 101 | 4.602E+01 | -1.280E+04 | 0 | 0 | 0 | 273.15 | 293.15 | < 100% | P |
| ANISOLE | 100-66-3 | 101 | 2.158E+01 | -4.179E+03 | 0 | 0 | 0 | 275.15 | 363.85 | < 5% | E |
| DIPHENYL ETHER | 101-84-8 | 100 | 2.903E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **OTHER INORGANICS** | | | | | | | | | | | |
| HYDROGEN PEROXIDE | 7722-84-1 | 101 | 2.142E+01 | -7.235E+03 | 0 | 0 | 0 | 278.15 | 297.15 | < 25% | E |
| **OTHER MONOAROMATICS** | | | | | | | | | | | |
| STYRENE | 100-42-5 | 101 | 2.190E+01 | -3.653E+03 | 0 | 0 | 0 | 293.32 | 313.02 | < 5% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER POLYFUNCTIONAL C, H, O** | | | | | | | | | | | |
| 2-BUTOXYETHANOL | 111-76-2 | 101 | 2.922E+01 | -8.275E+03 | 0 | 0 | 0 | 293.15 | 303.15 | < 25% | E |
| VANILLIN | 121-33-5 | 101 | -3.909E+02 | 1.144E+04 | 6.127E+01 | 0 | 0 | 293.15 | 318.15 | < 5% | E |
| **OTHER POLYFUNCTIONAL ORGANICS** | | | | | | | | | | | |
| MALATHION | 121-75-5 | 101 | 2.879E+01 | -8.274E+03 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| **OTHER SATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ISOVALERATE | 108-64-5 | 101 | 2.443E+02 | -1.600E+04 | -3.201E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| DIETHYL MALONATE | 105-53-3 | 101 | 2.731E+02 | -1.846E+04 | -3.660E+01 | 0 | 0 | 273.15 | 363.75 | < 10% | P |
| DIETHYL SUCCINATE | 123-25-1 | | | | | | | | | | |
| ETHYL TRIMETHYL ACETATE | 3938-95-2 | 101 | 2.619E+02 | -1.693E+04 | -3.441E+01 | 0 | 0 | 273.15 | 363.55 | < 25% | E |
| PEROXIDES | | | | | | | | | | | |
| METHYL HYDROPEROXIDE | 3031-73-0 | 101 | 2.049E+01 | -5.244E+03 | 0 | 0 | 0 | 277.15 | 297.15 | < 3% | E |
| ETHYL HYDROPEROXIDE | 3031-74-1 | 101 | 2.288E+01 | -5.985E+03 | 0 | 0 | 0 | 278.15 | 297.15 | < 10% | E |
| **POLYFUNCTIONAL AMIDES/AMINES** | | | | | | | | | | | |
| N,N-DIMETHYLFORMAMIDE | 68-12-2 | 101 | 2.051E+02 | -1.570E+04 | -2.692E+01 | 0 | 0 | 289.4 | 372 | < 25% | E |
| N-METHYLFORMAMIDE | 123-39-7 | 101 | 2.081E+01 | -7.161E+03 | 0 | 0 | 0 | 333.15 | 372.65 | < 5% | E |
| N,N-DIMETHYLACETAMIDE | 127-19-5 | 101 | 2.480E+01 | -8.014E+03 | 0 | 0 | 0 | 343.15 | 372.28 | < 10% | E |
| **POLYFUNCTIONAL C, H, N, HALIDE, (O)** | | | | | | | | | | | |
| o-CHLOROANILINE | 95-51-2 | 101 | 1.336E+03 | -5.042E+04 | -2.173E+02 | 2.501E-01 | 1 | 298.15 | 431.15 | < 25% | P |
| p-CHLORONITROBENZENE | 100-00-5 | 101 | 2.414E+01 | -5.868E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| **POLYFUNCTIONAL C, H, O, HALIDE** | | | | | | | | | | | |
| DI(2-CHLOROETHYL)ETHER | 111-44-4 | 101 | 2.107E+02 | -1.440E+04 | -2.767E+01 | 0 | 0 | 273.15 | 364.85 | < 5% | E |
| ETHYLCHLOROACETATE | 105-39-5 | 101 | 2.546E+02 | -1.630E+04 | -3.415E+01 | 0 | 0 | 273.15 | 333.25 | < 10% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| METHYL CHLOROACETATE | 96-34-4 | 101 | 1.755E+02 | -1.239E+04 | -2.268E+01 | 0 | 0 | 273.15 | 323.35 | < 5% | E |
| **POLYFUNCTIONAL C, H, O, N** | | | | | | | | | | | |
| N-METHYL-2-PYRROLIDONE | 872-50-4 | 101 | 4.600E+02 | -3.011E+04 | -6.372E+01 | 0 | 0 | 298.8 | 372.85 | < 5% | E |
| POLYFUNCTIONAL C, H, O, S | | | | | | | | | | | |
| DIMETHYL SULFOXIDE | 67-68-5 | 101 | 2.115E+01 | -7.789E+03 | 0 | 0 | 0 | 298.8 | 337.9 | < 25% | E |
| **POLYFUNCTIONAL ESTERS** | | | | | | | | | | | |
| METHYL SALICYLATE | 119-36-8 | 101 | 4.635E+02 | -2.852E+04 | -6.394E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| 2-ETHOXYETHYL ACETATE | 111-15-9 | 100 | 1.850E+01 | 0 | 0 | 0 | 0 | 303.15 | 303.15 | < 10% | E |
| ETHYL ACETOACETATE | 141-97-9 | 101 | 2.610E+01 | -7.239E+03 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | EP |
| ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 112-07-2 | 100 | 3.062E+01 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| **PROPIONATES AND BUTYRATES** | | | | | | | | | | | |
| METHYL PROPIONATE | 554-12-1 | 101 | 2.605E+01 | -5.719E+03 | 0 | 0 | 0 | 273.15 | 310.2 | < 5% | E |
| ETHYL PROPIONATE | 105-37-3 | 101 | 2.963E+02 | -1.786E+04 | -4.021E+01 | 0 | 0 | 273.15 | 353.45 | < 25% | E |
| n-PROPYL PROPIONATE | 106-36-5 | 101 | 2.299E+02 | -1.536E+04 | -2.996E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| n-BUTYL PROPIONATE | 590-01-2 | 101 | 2.785E+02 | -1.795E+04 | -3.694E+01 | 0 | 0 | 273.15 | 363.55 | < 10% | E |
| n-PROPYL n-BUTYRATE | 105-66-8 | 101 | 2.587E+02 | -1.660E+04 | -3.422E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| METHYL n-BUTYRATE | 623-42-7 | 101 | 1.665E+02 | -1.196E+04 | -2.091E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ETHYL n-BUTYRATE | 105-54-4 | 101 | 1.949E+02 | -1.355E+04 | -2.488E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ISOBUTYL ISOBUTYRATE | 97-85-8 | 101 | 2.887E+02 | -1.832E+04 | -3.832E+01 | 0 | 0 | 273.15 | 363.45 | < 25% | E |
| n-BUTYL n-BUTYRATE | 109-21-7 | 101 | 3.706E+02 | -2.260E+04 | -5.032E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| METHYL ISOBUTYRATE | 547-63-7 | 101 | 2.024E+02 | -1.347E+04 | -2.625E+01 | 0 | 0 | 273.15 | 353.45 | < 10% | E |
| ETHYL ISOBUTYRATE | 97-62-1 | 101 | 1.871E+02 | -1.308E+04 | -2.370E+01 | 0 | 0 | 273.15 | 363.75 | < 10% | P |
| n-PENTYL n-BUTYRATE | 540-18-1 | 101 | 2.955E+01 | -6.393E+03 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |

Table C.2: $k_H$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ISOPENTYL BUTYRATE | 106-27-4 | 101 | 3.076E+02 | -1.973E+04 | -4.087E+01 | 0 | 0 | 282.55 | 363.85 | < 100% | E |
| **SULFIDES/THIOPHENES** | | | | | | | | | | | |
| DIMETHYL SULFIDE | 75-18-3 | 101 | 2.083E+02 | -1.184E+04 | -2.797E+01 | 0 | 0 | 272.35 | 353.45 | < 10% | E |
| DIMETHYL DISULFIDE | 624-92-0 | 101 | 2.120E+01 | -3.695E+03 | 0 | 0 | 0 | 273.2 | 343.15 | < 10% | E |
| 2-METHYLTHIOPHENE | 554-14-3 | 101 | 2.390E+01 | -4.287E+03 | 0 | 0 | 0 | 298.15 | 343.15 | < 10% | E |
| DIISOPROPYL SULFIDE | 625-80-9 | 101 | 2.628E+01 | -4.889E+03 | 0 | 0 | 0 | 298.15 | 343.15 | < 10% | E |
| **UNSATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ACRYLATE | 140-88-5 | 101 | 2.199E+01 | -4.393E+03 | 0 | 0 | 0 | 298.6 | 360.2 | < 10% | P |
| METHYL METHACRYLATE | 80-62-6 | 101 | 2.853E+02 | -1.690E+04 | -3.880E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |

Table C.3: $\gamma_i^\infty$ regression summary

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **1-ALKENES** | | | | | | | | | | | |
| 1-PENTENE | 109-67-1 | 100 | 2.2033E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXENE | 592-41-6 | 100 | 9.1053E+04 | 4.5755E+03 | 5.6855E+00 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEPTENE | 592-76-7 | 100 | 3.7625E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-OCTENE | 111-66-0 | 100 | 1.5549E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-NONENE | 124-11-8 | 100 | 6.4250E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-DECENE | 872-05-9 | 100 | 2.6552E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-UNDECENE | 872-05-9 | 100 | 1.0973E+08 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-DODECENE | 872-05-9 | 100 | 4.5341E+08 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-TRIDECENE | 592-41-6 | 100 | 1.8737E+09 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-TETRADECENE | 872-05-9 | 100 | 7.7426E+09 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-PENTADECENE | 13360-61-7 | 100 | 3.1997E+10 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **2,3,4-ALKENES** | | | | | | | | | | | |
| cis-2-PENTENE | 627-20-3 | 100 | 1.9178E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| trans-2-PENTENE | 646-04-8 | 100 | 1.9178E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| cis-2-HEPTENE | 6443-92-1 | 100 | 3.6334E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| trans-2-HEPTENE | 14686-13-6 | 100 | 3.6334E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| **ACETATES** | | | | | | | | | | | |
| METHYL ACETATE | 79-20-9 | 101 | 4.0958E+02 | -1.9719E+04 | -5.9724E+01 | 0 | 0 | 293.15 | 343.25 | < 10% | E |
| ETHYL ACETATE | 141-78-6 | 101 | 1.8730E+02 | -9.2371E+03 | -2.6696E+01 | 0 | 0 | 288.15 | 353.15 | < 10% | E |
| n-PROPYL ACETATE | 109-60-4 | 101 | 2.2269E+02 | -1.0697E+04 | -3.1801E+01 | 0 | 0 | 298 | 343.25 | < 10% | E |
| n-BUTYL ACETATE | 123-86-4 | 101 | 1.7311E+02 | -8.2435E+03 | -2.4321E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| ISOBUTYL ACETATE | 110-19-0 | 101 | 2.9865E+01 | -1.9167E+03 | -2.9174E+00 | 0 | 0 | 273.15 | 323.15 | < 25% | E |
| ISOPENTYL ACETATE | 123-92-2 | 101 | 2.3843E+02 | -1.1153E+04 | -3.3853E+01 | 0 | 0 | 273.15 | 363.85 | < 10% | E |
| ISOPROPYL ACETATE | 108-21-4 | 101 | -1.0523E+02 | 3.4976E+03 | 1.7345E+01 | 0 | 0 | 273.15 | 310.2 | < 25% | E |
| sec-BUTYL ACETATE | 105-46-4 | 101 | 1.8364E+02 | -8.8655E+03 | -2.5835E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| VINYL ACETATE | 108-05-4 | 101 | 1.3344E+02 | -6.0176E+03 | -1.8964E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |
| n-PENTYL ACETATE | 628-63-7 | 101 | 3.3660E+02 | -1.5786E+04 | -4.8331E+01 | 0 | 0 | 273.15 | 364.5 | < 25% | E |
| n-HEXYL ACETATE | 142-92-7 | 101 | 3.7674E+02 | -1.7146E+04 | -5.4324E+01 | 0 | 0 | 273.15 | 363.35 | < 25% | E |
| n-HEPTYL ACETATE | 112-06-1 | 100 | 6.5861E+04 | -1.8462E+04 | -3.6599E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| n-OCTYL ACETATE | 112-14-1 | 100 | 2.6455E+05 | -2.1364E+04 | -4.5483E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| tert-BUTYL ACETATE | 540-88-5 | 101 | 1.6617E+02 | -8.2029E+03 | -2.3147E+01 | 0 | 0 | 273.15 | 353.65 | < 10% | E |
| CYCLOHEXYL ACETATE | 622-45-7 | 101 | 2.0341E+02 | -9.4699E+03 | -2.8728E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| PHENYL ACETATE | 122-79-2 | 101 | 1.6704E+02 | -7.1054E+03 | -2.3876E+01 | 0 | 0 | 273.15 | 363.95 | < 10% | E |
| **ALDEHYDES** | | | | | | | | | | | |
| PROPANAL | 123-38-6 | 101 | 2.3549E+02 | -1.1978E+04 | -3.3870E+01 | 0 | 0 | 278.15 | 318.15 | < 5% | E |
| BUTANAL | 123-72-8 | 101 | 1.0100E+01 | -1.9064E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| 2-METHYLPROPANAL | 78-84-2 | 100 | 5.1912E+01 | -6.5156E+03 | -2.1156E+01 | -8.2308E-06 | 2 | 298.15 | 298.15 | < 5% | S |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PENTANAL | 110-62-3 | 101 | 1.1248E+01 | -1.7998E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| HEPTANAL | 111-71-7 | 101 | 1.4484E+01 | -1.9125E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| HEXANAL | 66-25-1 | 101 | 1.0459E+01 | -1.1086E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| OCTANAL | 124-13-0 | 101 | 1.3249E+01 | -1.0346E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 10% | E |
| NONANAL | 124-19-6 | 101 | 8.9172E+00 | 8.7039E+02 | 0 | 0 | 0 | 283.15 | 318.15 | < 25% | E |
| 2-ETHYLHEXANAL | 123-05-7 | 101 | 8.2330E+00 | 4.5752E+02 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| 2-ETHYL-2-HEXENAL | 645-62-5 | 101 | 8.3085E+00 | 1.0122E+02 | 0 | 0 | 0 | 273.15 | 363.15 | < 50% | E |
| DECANAL | 112-31-2 | 101 | 1.6820E+01 | -1.0090E+03 | 0 | 0 | 0 | 298.15 | 318.15 | < 50% | E |
| 2-METHYL-BUTYRALDEHYDE | 96-17-3 | 101 | 9.8196E+00 | -1.2187E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | P |
| ACROLEIN | 107-02-8 | 101 | 7.9257E+00 | -1.4558E+03 | 0 | 0 | 0 | 273 | 298 | < 100% | E |
| trans-CROTONALDEHYDE | 123-73-9 | 101 | 1.2597E+02 | -5.9638E+03 | -1.8057E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | EP |
| METHACROLEIN | 78-85-3 | 101 | 6.5218E+00 | -7.1561E+02 | 0 | 0 | 0 | 273.15 | 333.15 | < 10% | E |
| p-TOLUALDEHYDE | 104-87-0 | 101 | 9.6622E+00 | -5.4954E+02 | 0 | 0 | 0 | 278 | 298 | < 25% | E |
| BENZALDEHYDE | 100-52-7 | 101 | 5.1540E+02 | -2.1901E+04 | -7.6382E+01 | 0 | 0 | 273.08 | 323.15 | < 10% | E |
| m-TOLUALDEHYDE | 620-23-5 | 101 | 9.4640E+00 | -3.8418E+02 | 0 | 0 | 0 | 278 | 298 | < 25% | E |
| **ALIPHATIC ETHERS** | | | | | | | | | | | |
| DIETHYL ETHER | 60-29-7 | 101 | 2.3981E+02 | -1.2537E+04 | -3.3940E+01 | 0 | 0 | 273.35 | 333.25 | < 5% | E |
| DIISOPROPYL ETHER | 108-20-3 | 101 | -4.6536E+01 | 7.2880E+01 | 9.2540E+00 | 0 | 0 | 273.15 | 334.15 | < 10% | E |
| DI-n-BUTYL ETHER | 142-96-1 | 101 | 1.4973E+01 | -1.3729E+03 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| METHYL tert-BUTYL ETHER | 1634-04-4 | 101 | 5.7408E+01 | -4.2388E+03 | -6.7324E+00 | 0 | 0 | 273.15 | 343.15 | < 10% | E |
| METHYL ISOBUTYL ETHER | 625-44-5 | 101 | 1.5503E+01 | -2.8030E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 5% | E |
| DI-n-HEXYL ETHER | 112-58-3 | 100 | 1.4510E+07 | -1.8280E+04 | -5.4709E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| METHYL n-BUTYL ETHER | 628-28-4 | 101 | 7.0311E+02 | -3.2841E+04 | -1.0296E+02 | 0 | 0 | 273.15 | 298.15 | < 25% | E |
| DI-n-PENTYL ETHER | 693-65-2 | 100 | 4.5100E+05 | -7.0534E+03 | -2.2745E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| METHYL tert-PENTYL ETHER | 994-05-8 | 101 | 1.7808E+02 | -9.7068E+03 | -2.4430E+01 | 0 | 0 | 273.15 | 352.35 | < 10% | E |
| tert-BUTYL ETHYL ETHER | 637-92-3 | 101 | 1.5616E+01 | -2.8259E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| ETHYL tert-PENTYL ETHER | 919-94-8 | 101 | 1.7640E+01 | -2.9893E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| DI-n-PROPYL ETHER | 111-43-3 | 101 | 4.0286E+02 | -1.9387E+04 | -5.7942E+01 | 0 | 0 | 273.15 | 333.25 | < 5% | E |
| n-BUTYL ETHYL ETHER | 628-81-9 | 101 | 2.0852E+02 | -1.0117E+04 | -2.9431E+01 | 0 | 0 | 273.15 | 363.85 | < 25% | E |
| ALKYLCYCLOHEXANES | | | | | | | | | | | |
| METHYLCYCLOHEXANE | 108-87-2 | 101 | 3.6535E+02 | -1.5923E+04 | -5.2511E+01 | 0 | 0 | 293.15 | 443.95 | < 25% | E |
| ETHYLCYCLOHEXANE | 1678-91-7 | 101 | 1.7556E+03 | -5.4303E+04 | -2.9260E+02 | 3.6218E-01 | 1 | 273.15 | 443.95 | < 10% | E |
| cis-1,2-DIMETHYL-CYCLOHEXANE | 2207-01-4 | 101 | 3.3288E+02 | -1.3995E+04 | -4.7754E+01 | 0 | 0 | 273.15 | 313.15 | < 25% | E |
| trans-1,2-DIMETHYL-CYCLOHEXANE | 6876-23-9 | 101 | 1.4668E+03 | -4.6285E+04 | -2.4271E+02 | 2.8645E-01 | 1 | 273.15 | 443.25 | < 5% | E |
| **ALKYLCYCLOPENTANES** | | | | | | | | | | | |
| METHYL-CYCLOPENTANE | 96-37-7 | 100 | 1.0935E+05 | -7.8306E+03 | -2.7270E+01 | -6.3208E-06 | 2 | 298.15 | 298.15 | < 3% | S |
| **ALKYNES** | | | | | | | | | | | |
| 1-PENTYNE | 627-19-0 | 100 | 2.4720E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXYNE | 693-02-7 | 100 | 1.1810E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-OCTYNE | 629-05-0 | 100 | 2.5340E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-NONYNE | 3452-09-3 | 100 | 1.3100E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEPTYNE | 628-71-7 | 100 | 5.4810E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **AROMATIC ALCOHOLS** | | | | | | | | | | | |
| 2,3-XYLENOL | 526-75-0 | 101 | 3.2073E+00 | 9.3895E+02 | 0 | 0 | 0 | 349.05 | 371.65 | < 25% | S |
| 2,4-XYLENOL | 105-67-9 | 101 | 1.6630E+00 | 1.5325E+03 | 0 | 0 | 0 | 349.05 | 371.65 | < 25% | E |
| 2,5-XYLENOL | 95-87-4 | 101 | 3.4136E+02 | -1.5740E+04 | -4.9567E+01 | 0 | 0 | 278 | 371.65 | < 10% | E |
| 2,6-XYLENOL | 576-26-1 | 101 | 1.2864E+02 | -4.9837E+03 | -1.8451E+01 | 0 | 0 | 278 | 371.65 | < 10% | E |
| 3,4-XYLENOL | 95-65-8 | 101 | 3.2111E+00 | 8.9290E+02 | 0 | 0 | 0 | 293.15 | 371.65 | < 25% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3,5-XYLENOL | 108-68-9 | 101 | 1.1755E+02 | -4.5606E+03 | -1.6823E+01 | 0 | 0 | 293.15 | 371.65 | < 25% | E |
| PHENOL | 108-95-2 | 101 | 4.5472E+02 | -2.1677E+04 | -6.6388E+01 | 0 | 0 | 278 | 373.15 | < 25% | E |
| o-CRESOL | 95-48-7 | 101 | 2.1997E+02 | -9.7201E+03 | -3.1956E+01 | 0 | 0 | 293.15 | 371.65 | < 5% | E |
| m-CRESOL | 108-39-4 | 101 | -1.5582E+01 | 2.1554E+03 | 2.4416E+00 | 0 | 0 | 298.15 | 371.65 | < 25% | E |
| p-CRESOL | 106-44-5 | 101 | 1.5458E+02 | -6.2545E+03 | -2.2485E+01 | 0 | 0 | 298 | 371.65 | < 3% | E |
| 2-PHENYLETHANOL | 60-12-8 | 101 | 1.7589E+02 | -7.4876E+03 | -2.5479E+01 | 0 | 0 | 283.15 | 373.15 | < 10% | P |
| **AROMATIC AMINES** | | | | | | | | | | | |
| o-TOLUIDINE | 95-53-4 | 101 | 5.6946E+00 | 3.2271E+01 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |
| m-TOLUIDINE | 108-44-1 | 101 | 5.6591E+00 | 8.1355E+01 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |
| p-TOLUIDINE | 106-49-0 | 101 | 6.3431E-01 | 1.6356E+03 | 0 | 0 | 0 | 293.15 | 313.15 | < 5% | P |
| N,N-DIETHYLANILINE | 91-66-7 | 101 | 9.2931E+00 | 4.2183E+02 | 0 | 0 | 0 | 273.15 | 333.15 | < 25% | E |
| PYRIDINE | 110-86-1 | 101 | 3.2354E+00 | -4.9087E+01 | 0 | 0 | 0 | 298 | 374.15 | < 25% | E |
| ANILINE | 62-53-3 | 101 | 1.8127E+02 | -8.1850E+03 | -2.6142E+01 | 0 | 0 | 298 | 374.15 | < 10% | E |
| 2-METHYLPYRIDINE | 109-06-8 | 101 | 7.8877E+00 | -1.2722E+03 | 0 | 0 | 0 | 298 | 313.15 | < 5% | E |
| o-ETHYLANILINE | 578-54-1 | 101 | 1.6012E+02 | -7.0534E+03 | -2.2745E+01 | 0 | 0 | 283.15 | 363.15 | < 10% | P |
| 2,6-DIMETHYLPYRIDINE | 108-48-5 | 101 | 1.1003E+01 | -1.9828E+03 | 0 | 0 | 0 | 298 | 313.15 | < 25% | E |
| 3-METHYLPYRIDINE | 108-99-6 | 101 | 7.5009E+00 | -1.0441E+03 | 0 | 0 | 0 | 298 | 313.15 | < 25% | E |
| 4-METHYLPYRIDINE | 108-89-4 | 101 | 7.6057E+00 | -1.1383E+03 | 0 | 0 | 0 | 298 | 313.15 | < 5% | E |
| 2,4-DIMETHYLANILINE | 95-68-1 | 101 | 2.6650E+02 | -1.2031E+04 | -3.8444E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | P |
| N-ETHYLANILINE | 103-69-5 | 101 | 1.8651E+02 | -8.4052E+03 | -2.6420E+01 | 0 | 0 | 273.15 | 363.15 | < 10% | E |
| **AROMATIC CHLORIDES** | | | | | | | | | | | |
| BENZYL CHLORIDE | 100-44-7 | 101 | 4.7978E+00 | 1.4249E+03 | 0 | 0 | 0 | 277.65 | 303.15 | < 25% | E |
| MONOCHLOROBENZENE | 108-90-7 | 101 | 3.0084E+02 | -1.1883E+04 | -4.4139E+01 | 0 | 0 | 274.15 | 353.16 | < 10% | E |
| o-DICHLOROBENZENE | 95-50-1 | 101 | 7.4286E+02 | -3.1963E+04 | -1.0964E+02 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| m-DICHLOROBENZENE | 541-73-1 | 101 | 7.3203E+00 | 1.1112E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| p-DICHLOROBENZENE | 106-46-7 | 101 | 5.2227E+02 | -2.3008E+04 | -7.6204E+01 | 0 | 0 | 278.15 | 346.55 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| HEXACHLOROBENZENE | 118-74-1 | 101 | 9.4803E+00 | 2.8438E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| o-CHLOROTOLUENE | 95-49-8 | 101 | 7.5502E+00 | 9.9128E+02 | 0 | 0 | 0 | 274.15 | 318.15 | < 25% | E |
| p-CHLOROTOLUENE | 106-43-4 | 101 | 7.8721E+00 | 9.0900E+02 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 2,4-DICHLOROTOLUENE | 95-73-8 | 101 | 8.0122E+00 | 1.4043E+03 | 0 | 0 | 0 | 278.15 | 323.1 | < 10% | E |
| 1,2,4-TRICHLOROBENZENE | 120-82-1 | 101 | 1.0415E+01 | 6.0490E+02 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 1,2,3-TRICHLOROBENZENE | 87-61-6 | 101 | 6.1575E+00 | 1.9216E+03 | 0 | 0 | 0 | 277.15 | 323.15 | < 25% | E |
| **AROMATIC ESTERS** | | | | | | | | | | | |
| BENZYL ACETATE | 140-11-4 | 101 | 7.1499E+00 | 2.6685E+02 | 0 | 0 | 0 | 273.15 | 322.95 | < 25% | E |
| DI-n-PROPYL PHTHALATE | 131-16-8 | 100 | 1.5080E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DI-n-HEXYL PHTHALATE | 84-75-3 | 100 | 7.9098E+07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| METHYL BENZOATE | 93-58-3 | 101 | 1.9660E+02 | -8.1145E+03 | -2.8291E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ETHYL BENZOATE | 93-89-0 | 101 | 1.4804E+02 | -6.1565E+03 | -2.0767E+01 | 0 | 0 | 273.15 | 363.45 | < 25% | E |
| BENZYL FORMATE | 104-57-4 | 101 | 7.6942E+00 | -3.4741E+02 | 0 | 0 | 0 | 273.15 | 322.85 | < 25% | E |
| DIETHYL PHTHALATE | 84-66-2 | 101 | 2.9610E+02 | -1.2896E+04 | -4.2710E+01 | 0 | 0 | 278.15 | 374.15 | < 10% | E |
| DI-n-BUTYL PHTHALATE | 84-74-2 | 101 | 7.8577E+02 | -3.4556E+04 | -1.1507E+02 | 0 | 0 | 283.15 | 323.15 | < 25% | E |
| DIMETHYL PHTHALATE | 131-11-3 | 101 | 2.1362E+02 | -8.7600E+03 | -3.0969E+01 | 0 | 0 | 283.15 | 374.15 | < 10% | EP |
| **C, H, BR COMPOUNDS** | | | | | | | | | | | |
| BROMOETHANE | 74-96-4 | 101 | 7.9924E+00 | -4.4577E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 3% | E |
| 1,1,2,2-TETRABROMOETHANE | 79-27-6 | 101 | -7.0038E+00 | 6.0714E+03 | 0 | 0 | 0 | 298.15 | 323.15 | < 50% | E |
| 1-BROMOPROPANE | 106-94-5 | 101 | 9.9920E+00 | -6.0960E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| 2-BROMOPROPANE | 75-26-3 | 101 | 3.4368E+02 | -1.5159E+04 | -5.0051E+01 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| 1-BROMOBUTANE | 109-65-9 | 100 | 1.3502E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-BROMOHEPTANE | 629-04-9 | 100 | 1.3438E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1,2-DIBROMOETHANE | 106-93-4 | 101 | 6.1031E+00 | 4.9221E+02 | 0 | 0 | 0 | 273.15 | 363.75 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| m-DIBROMOBENZENE | 108-36-1 | 100 | 1.3275E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| BROMOBENZENE | 108-86-1 | 101 | 3.9706E+02 | -1.6495E+04 | -5.8226E+01 | 0 | 0 | 283.15 | 343.15 | < 10% | E |
| TRIBROMOMETHANE | 75-25-2 | 101 | 6.8448E+00 | 4.4238E+02 | 0 | 0 | 0 | 283 | 313.15 | < 10% | E |
| DIBROMOMETHANE | 74-95-3 | 101 | 6.9877E+01 | -2.6491E+03 | -9.5301E+00 | 0 | 0 | 273.15 | 363.25 | < 5% | E |
| 2-BROMOBUTANE | 78-76-2 | 100 | 8.3200E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| p-BROMOTOLUENE | 106-38-7 | 101 | 8.7771E+00 | 7.6479E+02 | 0 | 0 | 0 | 293.1 | 322.91 | < 25% | E |
| **C, H, F COMPOUNDS** | | | | | | | | | | | |
| PERFLUORO-n-HEXANE | 355-42-0 | 100 | 2.0497E+08 | 1.2453E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-OCTANE | 307-34-6 | 100 | 1.4564E+10 | -3.7208E+04 | -1.0276E+02 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| 1,2-DIFLUOROBENZENE | 367-11-3 | 101 | 6.6988E+00 | 5.9091E+02 | 0 | 0 | 0 | 298.15 | 322.89 | < 25% | E |
| FLUOROBENZENE | 462-06-6 | 101 | 1.4087E+02 | -5.8074E+03 | -1.9867E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | E |
| HEXAFLUOROBENZENE | 392-56-3 | 101 | 2.7504E+02 | -1.2435E+04 | -3.9248E+01 | 0 | 0 | 281.46 | 339.76 | < 3% | E |
| PERFLUORO-n-PENTANE | 678-26-2 | 100 | 1.3835E+07 | 7.9863E+01 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-HEPTANE | 335-57-9 | 100 | 1.7852E+09 | -6.8024E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| **C, H, I COMPOUNDS** | | | | | | | | | | | |
| METHYL IODIDE | 74-88-4 | 101 | 3.2179E+02 | -1.3816E+04 | -4.7240E+01 | 0 | 0 | 273.15 | 322.91 | < 5% | E |
| ETHYL IODIDE | 75-03-6 | 101 | 2.9938E+02 | -1.2802E+04 | -4.3660E+01 | 0 | 0 | 273.15 | 303.15 | < 3% | E |
| n-PROPYL IODIDE | 107-08-4 | 101 | 9.8486E+00 | -2.1844E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| ISOPROPYL IODIDE | 75-30-9 | 101 | 1.0634E+01 | -5.3563E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| IODOBENZENE | 591-50-4 | 101 | -1.6323E+01 | 8.1025E+03 | 0 | 0 | 0 | 298 | 303.15 | < 25% | E |
| n-HEXYL IODIDE | 638-45-9 | 100 | 8.3652E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| n-BUTYL IODIDE | 542-69-8 | 100 | 4.3976E+04 | -1.3108E+04 | -5.1464E+01 | 4.2552E-02 | 1 | 298.15 | 298.15 | < 25% | S |
| **C, H, MULTIHALOGEN COMPOUNDS** | | | | | | | | | | | |
| 1,1,2-TRICHLOROTRIFLUORO-ETHANE | 76-13-1 | 101 | 1.2459E+01 | -5.4053E+02 | 0 | 0 | 0 | 275.15 | 303.15 | < 25% | E |
| | | | | | | | | | | | |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **C, H, NO2 COMPOUNDS** | | | | | | | | | | | |
| NITROMETHANE | 75-52-5 | 101 | 1.9786E+02 | -8.0194E+03 | -2.9403E+01 | 0 | 0 | 273.15 | 363.15 | < 10% | E |
| NITROETHANE | 79-24-3 | 101 | 1.1679E+02 | -4.7515E+03 | -1.6904E+01 | 0 | 0 | 273.15 | 363.25 | < 5% | E |
| 1-NITROPROPANE | 108-03-2 | 101 | 1.4552E+02 | -6.1723E+03 | -2.0902E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| 2-NITROPROPANE | 79-46-9 | 101 | 1.1132E+02 | -4.6173E+03 | -1.5829E+01 | 0 | 0 | 292.85 | 363.35 | < 3% | E |
| 1-NITROBUTANE | 627-05-4 | 100 | 1.5314E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| o-NITROTOLUENE | 88-72-2 | 101 | 5.7392E+00 | 1.0851E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| p-NITROTOLUENE | 99-99-0 | 101 | 7.6320E+00 | 5.3380E+02 | 0 | 0 | 0 | 281 | 338 | < 10% | E |
| m-NITROTOLUENE | 99-08-1 | 101 | 8.8637E+00 | 2.1248E+02 | 0 | 0 | 0 | 283.15 | 313.15 | < 25% | E |
| NITROBENZENE | 98-95-3 | 101 | 1.4633E+02 | -5.4696E+03 | -2.1029E+01 | 0 | 0 | 283.15 | 372.85 | < 5% | E |
| 2,4-DINITROTOLUENE | 121-14-2 | 101 | 3.5728E+02 | -1.4679E+04 | -5.2362E+01 | 0 | 0 | 277.15 | 334.95 | < 5% | E |
| 2,6-DINITROTOLUENE | 606-20-2 | 101 | 2.5130E-02 | 2.9932E+03 | 0 | 0 | 0 | 278 | 314 | < 5% | E |
| 3,4-DINITROTOLUENE | 610-39-9 | 101 | 4.9257E+00 | 1.5634E+03 | 0 | 0 | 0 | 278.2 | 313.2 | < 5% | E |
| 2,4,6-TRINITROTOLUENE | 118-96-7 | 101 | 4.9257E+02 | -2.0991E+04 | -7.2348E+01 | 0 | 0 | 275.55 | 334.15 | < 10% | E |
| **C1/C2 ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| CARBON TETRACHLORIDE | 56-23-5 | 101 | 3.2892E+02 | -1.4418E+04 | -4.7608E+01 | 0 | 0 | 273.15 | 366.15 | < 5% | E |
| DICHLOROMETHANE | 75-09-2 | 101 | 7.7957E+01 | -2.9989E+03 | -1.0948E+01 | 0 | 0 | 273.15 | 366.15 | < 10% | E |
| CHLOROFORM | 67-66-3 | 101 | 1.7864E+02 | -7.9325E+03 | -2.5502E+01 | 0 | 0 | 273.15 | 366.15 | < 3% | E |
| 1,1-DICHLOROETHANE | 75-34-3 | 101 | 2.1919E+02 | -9.6308E+03 | -3.1578E+01 | 0 | 0 | 273.15 | 366.15 | < 5% | E |
| 1,2-DICHLOROETHANE | 107-06-2 | 101 | 2.2719E+02 | -9.8351E+03 | -3.2955E+01 | 0 | 0 | 273.15 | 366.15 | < 10% | E |
| 1,1,2-TRICHLOROETHANE | 79-00-5 | 101 | 7.0028E+01 | -2.5094E+03 | -9.5188E+00 | 0 | 0 | 273.15 | 363.95 | < 5% | E |
| HEXACHLOROETHANE | 67-72-1 | 101 | 1.0718E+01 | 3.8043E+02 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| 1,1,1-TRICHLOROETHANE | 71-55-6 | 101 | 2.9839E+01 | -1.0774E+03 | -3.0848E+00 | 0 | 0 | 273.15 | 348.15 | < 10% | E |
| 1,1,1,2-TETRACHLOROETHANE | 630-20-6 | 101 | 8.5450E+00 | 1.3991E+02 | 0 | 0 | 0 | 273.15 | 323.15 | < 10% | E |
| | | | | | | | | | | | |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1,1,2,2-TETRACHLOROETHANE | 79-34-5 | 101 | 7.0902E+00 | 2.8054E+02 | 0 | 0 | 0 | 283.15 | 328.65 | < 10% | E |
| TRICHLOROETHYLENE | 79-01-6 | 101 | 2.2817E+02 | -9.8609E+03 | -3.2730E+01 | 0 | 0 | 274.22 | 366.15 | < 5% | E |
| TETRACHLORO-ETHYLENE | 127-18-4 | 101 | 2.6382E+02 | -1.1250E+04 | -3.7821E+01 | 0 | 0 | 273.15 | 364.95 | < 10% | E |
| cis-1,2-DICHLOROETHYLENE | 156-59-2 | 101 | 1.7602E+02 | -7.7385E+03 | -2.5154E+01 | 0 | 0 | 281.15 | 366.15 | < 10% | E |
| trans-1,2-DICHLOROETHYLENE | 156-60-5 | 101 | 8.5045E+00 | -4.1902E+02 | 0 | 0 | 0 | 283.15 | 323.15 | < 10% | E |
| PENTACHLOROETHANE | 76-01-7 | 101 | 1.7025E+01 | -2.0327E+03 | 0 | 0 | 0 | 293.15 | 298 | < 25% | E |
| 1,1-DICHLOROETHYLENE | 75-35-4 | 101 | 2.6075E+02 | -1.1818E+04 | -3.7462E+01 | 0 | 0 | 275.15 | 363.65 | < 10% | E |
| **C3 & HIGHER ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| 1,4-DICHLOROBUTANE | 110-56-5 | 101 | 2.1338E+00 | 1.9316E+03 | 0 | 0 | 0 | 286.65 | 298.05 | < 10% | E |
| 1,5-DICHLOROPENTANE | 628-76-2 | 101 | 3.5460E+00 | 2.1016E+03 | 0 | 0 | 0 | 274.15 | 295.85 | < 50% | E |
| 1,2-DICHLOROPROPANE | 78-87-5 | 101 | 2.1117E+02 | -8.8441E+03 | -3.0497E+01 | 0 | 0 | 273.15 | 353.35 | < 10% | E |
| ISOPROPYL CHLORIDE | 75-29-6 | 101 | 1.0546E+01 | -9.8481E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 10% | E |
| 1,2,3-TRICHLOROPROPANE | 96-18-4 | 101 | -4.0021E+00 | 3.6230E+03 | 0 | 0 | 0 | 275.05 | 318.15 | < 25% | E |
| HEXACHLORO-1,3-BUTADIENE | 87-68-3 | 101 | 1.0004E+01 | 1.4831E+03 | 0 | 0 | 0 | 275.15 | 298.15 | < 50% | E |
| PROPYL CHLORIDE | 540-54-5 | 101 | 1.0409E+01 | -9.0691E+02 | 0 | 0 | 0 | 273.15 | 310.15 | < 10% | E |
| n-BUTYL CHLORIDE | 109-69-3 | 101 | 1.0006E+01 | -3.3086E+02 | 0 | 0 | 0 | 273.35 | 310.15 | < 10% | E |
| sec-BUTYL CHLORIDE | 78-86-4 | 101 | 1.1007E+01 | -6.6744E+02 | 0 | 0 | 0 | 275.05 | 298.05 | < 10% | E |
| 1-CHLOROPENTANE | 543-59-9 | 101 | 3.5428E+02 | -1.4816E+04 | -5.1650E+01 | 0 | 0 | 275.65 | 310.15 | < 5% | E |
| 1,3-DICHLOROPROPANE | 142-28-9 | 101 | 2.5176E+00 | 1.6023E+03 | 0 | 0 | 0 | 275.05 | 303.15 | < 25% | E |
| **CYCLOALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| CYCLOHEXANOL | 108-93-0 | 101 | 5.9244E+00 | -2.8428E+02 | 0 | 0 | 0 | 298 | 333.15 | < 25% | E |
| **CYCLOALKANES** | | | | | | | | | | | |
| CYCLOPENTANE | 287-92-3 | 101 | 1.9711E+02 | -8.3807E+03 | -2.7898E+01 | 0 | 0 | 298 | 426.25 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| CYCLOHEXANE | 110-82-7 | 101 | -1.5818E+03 | 4.1569E+04 | 2.7982E+02 | -4.7222E-01 | 1 | 274.25 | 424.15 | < 25% | E |
| CYCLOHEPTANE | 291-64-5 | 100 | 2.8396E+05 | -1.1604E+04 | -3.5685E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| CYCLOOCTANE | 292-64-8 | 101 | 1.4629E+02 | -5.4727E+03 | -2.0027E+01 | 0 | 0 | 273.15 | 313.15 | < 10% | E |
| **CYCLOALKENES** | | | | | | | | | | | |
| CYCLOPENTENE | 142-29-0 | 101 | 8.1479E+00 | 1.4497E+02 | 0 | 0 | 0 | 283.15 | 298.15 | < 50% | E |
| CYCLOHEXENE | 110-83-8 | 101 | 8.1071E+00 | 4.6844E+02 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| CYCLOHEPTENE | 628-92-2 | 100 | 8.0884E+04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| CYCLOOCTENE | 931-88-4 | 101 | 1.4403E+02 | -5.2275E+03 | -2.0010E+01 | 0 | 0 | 273.15 | 313.15 | < 5% | E |
| **DIALKENES** | | | | | | | | | | | |
| 1,4-CYCLOHEXADIENE | 628-41-1 | 101 | 7.5073E+00 | 2.9784E+02 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| **DIMETHYLALKANES** | | | | | | | | | | | |
| 2,2-DIMETHYLBUTANE | 75-83-2 | 100 | 2.2886E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 2,3-DIMETHYLBUTANE | 79-29-8 | 101 | 3.5524E+02 | -1.5943E+04 | -5.0796E+01 | 0 | 0 | 273.15 | 422.65 | < 25% | E |
| 2,4-DIMETHYLPENTANE | 108-08-7 | 100 | 1.4765E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| 3,3-DIMETHYLPENTANE | 562-49-2 | 101 | -1.9290E+03 | 5.3299E+04 | 3.3822E+02 | -5.4678E-01 | 1 | 298.15 | 423.64 | < 25% | E |
| 2,2-DIMETHYLHEXANE | 590-73-8 | 101 | 6.2123E+02 | -2.6996E+04 | -9.0435E+01 | 0 | 0 | 273.15 | 313.15 | < 5% | E |
| 2,5-DIMETHYLHEXANE | 592-13-2 | 101 | 7.3845E+02 | -3.1648E+04 | -1.0825E+02 | 0 | 0 | 273.15 | 313.15 | < 3% | E |
| **DIPHENYL/POLYAROMATICS** | | | | | | | | | | | |
| BIPHENYL | 92-52-4 | 101 | 5.6749E+02 | -2.3787E+04 | -8.3311E+01 | 0 | 0 | 293.15 | 337.65 | < 10% | E |
| **EPOXIDES** | | | | | | | | | | | |
| 1,4-DIOXANE | 123-91-1 | 101 | 8.2490E+01 | -4.7383E+03 | -1.1380E+01 | 0 | 0 | 273.35 | 374.15 | < 25% | E |
| TETRAHYDROPYRAN | 142-68-7 | 101 | 1.7525E+02 | -9.0201E+03 | -2.4698E+01 | 0 | 0 | 273.35 | 328.15 | < 5% | E |
| TETRAHYDROFURAN | 109-99-9 | 101 | 8.7722E+00 | -1.7620E+03 | 0 | 0 | 0 | 273.35 | 328.15 | < 10% | E |
| DIBENZOFURAN | 132-64-9 | 101 | 7.8758E+00 | 1.5796E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| **FORMATES** | | | | | | | | | | | |
| METHYL FORMATE | 107-31-3 | 101 | 3.9227E+00 | -3.2472E+02 | 0 | 0 | 0 | 285.65 | 333.25 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ETHYL FORMATE | 109-94-4 | 101 | 4.6479E+00 | -2.0861E+02 | 0 | 0 | 0 | 293.15 | 333.25 | < 25% | E |
| n-PROPYL FORMATE | 110-74-7 | 101 | 6.5884E+00 | -4.3744E+02 | 0 | 0 | 0 | 272.15 | 333.15 | < 10% | E |
| n-BUTYL FORMATE | 592-84-7 | 101 | 3.0690E+00 | 9.7352E+02 | 0 | 0 | 0 | 273.15 | 363.75 | < 25% | E |
| ISOBUTYL FORMATE | 542-55-2 | 101 | 8.8201E+00 | -7.1323E+02 | 0 | 0 | 0 | 273.15 | 333.55 | < 10% | E |
| n-PENTYL FORMATE | 638-49-3 | 101 | 1.9856E+02 | -8.9809E+03 | -2.8183E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| tert-BUTYL FORMATE | 762-75-4 | 101 | 3.8562E+00 | 5.9690E+02 | 0 | 0 | 0 | 278.15 | 308.15 | < 5% | E |
| **KETONES** | | | | | | | | | | | |
| ACETONE | 67-64-1 | 101 | 9.4580E+01 | -5.3679E+03 | -1.3112E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| METHYL ETHYL KETONE | 78-93-3 | 101 | 1.8127E+02 | -9.1056E+03 | -2.5894E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 3-PENTANONE | 96-22-0 | 101 | 1.9745E+02 | -9.7433E+03 | -2.8115E+01 | 0 | 0 | 273.15 | 310.2 | < 10% | E |
| METHYL ISOBUTYL KETONE | 108-10-1 | 101 | 1.6218E+02 | -8.0097E+03 | -2.2744E+01 | 0 | 0 | 273.15 | 363.55 | < 10% | E |
| 3-HEPTANONE | 106-35-4 | 101 | 1.5436E+02 | -7.6036E+03 | -2.1344E+01 | 0 | 0 | 273.15 | 363.25 | < 10% | E |
| 4-HEPTANONE | 123-19-3 | 101 | 2.0951E+02 | -1.0110E+04 | -2.9533E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | E |
| 3-HEXANONE | 589-38-8 | 101 | 1.2634E+01 | -1.9968E+03 | 0 | 0 | 0 | 293.15 | 310.2 | < 10% | E |
| 2-PENTANONE | 107-87-9 | 101 | 1.6360E+02 | -8.2048E+03 | -2.3100E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| METHYL ISOPROPYL KETONE | 563-80-4 | 101 | 2.3714E+02 | -1.1611E+04 | -3.4030E+01 | 0 | 0 | 265.15 | 453.15 | < 10% | P |
| 2-HEXANONE | 591-78-6 | 101 | 7.9859E+01 | -4.3728E+03 | -1.0415E+01 | 0 | 0 | 273.15 | 312.75 | < 10% | E |
| 2-HEPTANONE | 110-43-0 | 101 | 2.2170E+02 | -1.0473E+04 | -3.1457E+01 | 0 | 0 | 273.15 | 363.65 | < 5% | P |
| 5-METHYL-2-HEXANONE | 110-12-3 | 101 | 2.2974E+02 | -1.0897E+04 | -3.2652E+01 | 0 | 0 | 273.15 | 362.85 | < 5% | P |
| 3,3-DIMETHYL-2-BUTANONE | 75-97-8 | 101 | 1.1488E+02 | -5.8789E+03 | -1.5707E+01 | 0 | 0 | 273.15 | 363.35 | < 5% | E |
| DIISOBUTYL KETONE | 108-83-8 | 101 | 2.7411E+02 | -1.2906E+04 | -3.8780E+01 | 0 | 0 | 273.15 | 363.85 | < 10% | E |
| DIISOPROPYL KETONE | 565-80-0 | 101 | 1.2060E+02 | -6.0752E+03 | -1.6336E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| 5-NONANONE | 502-56-7 | 101 | 2.1399E+02 | -1.0276E+04 | -2.9794E+01 | 0 | 0 | 273.15 | 363.75 | < 25% | E |
| 2-NONANONE | 821-55-6 | 101 | 2.6336E+02 | -1.2150E+04 | -3.7302E+01 | 0 | 0 | 273.15 | 364.35 | < 25% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ACETYLACETONE | 123-54-6 | 101 | 3.0614E-01 | 1.0727E+03 | 0 | 0 | 0 | 303.15 | 373.15 | < 25% | E |
| CYCLOPENTANONE | 120-92-3 | 101 | 6.5404E+00 | -9.4122E+02 | 0 | 0 | 0 | 293.2 | 353.15 | < 100% | E |
| CYCLOHEXANONE | 108-94-1 | 101 | 7.8156E+00 | -1.0863E+03 | 0 | 0 | 0 | 298 | 353.15 | < 10% | E |
| 2-OCTANONE | 111-13-7 | 101 | 2.7138E+02 | -1.3009E+04 | -3.8461E+01 | 0 | 0 | 273.15 | 364.15 | < 25% | E |
| ACETOPHENONE | 98-86-2 | 101 | 1.6261E+02 | -7.9720E+03 | -2.2643E+01 | 0 | 0 | 278 | 318.15 | < 25% | E |
| 3-OCTANONE | 106-68-3 | 101 | 1.3269E+02 | -6.2786E+03 | -1.8085E+01 | 0 | 0 | 273.15 | 364.15 | < 10% | E |
| 3-NONANONE | 925-78-0 | 101 | 9.4835E+00 | 5.2588E+01 | 0 | 0 | 0 | 273.15 | 353.35 | < 25% | E |
| 2,6,8-TRIMETHYL-4-NONANONE | 123-18-2 | 100 | 4.5321E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| **MERCAPTANS** | | | | | | | | | | | |
| ISOPROPYL MERCAPTAN | 75-33-2 | 101 | 7.2632E+00 | -6.7794E+01 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| n-BUTYL MERCAPTAN | 109-79-5 | 101 | 3.4604E+02 | -1.4901E+04 | -5.0435E+01 | 0 | 0 | 288.15 | 333.15 | < 10% | E |
| **METHYLALKANES** | | | | | | | | | | | |
| 2-METHYLPENTANE | 107-83-5 | 101 | 3.6405E+02 | -1.6321E+04 | -5.2063E+01 | 0 | 0 | 273.15 | 422.65 | < 25% | E |
| 3-METHYLPENTANE | 96-14-0 | 100 | 3.6949E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 3% | S |
| 2-METHYLHEXANE | 591-76-4 | 100 | 2.1898E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 3-METHYLHEXANE | 589-34-4 | 100 | 2.0958E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 3-METHYLHEPTANE | 589-81-1 | 100 | 8.0059E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| 4-METHYLHEPTANE | 589-53-7 | 100 | 7.5617E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| **N-ALCOHOLS** | | | | | | | | | | | |
| METHANOL | 67-56-1 | 101 | 5.6961E+01 | -3.1424E+03 | -8.0557E+00 | 0 | 0 | 273 | 373.15 | < 10% | E |
| ETHANOL | 64-17-5 | 101 | 1.1923E+02 | -6.2620E+03 | -1.6999E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-PROPANOL | 71-23-8 | 101 | 1.4622E+02 | -7.4561E+03 | -2.0812E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-BUTANOL | 71-36-3 | 101 | 2.2282E+02 | -1.0659E+04 | -3.2139E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 1-PENTANOL | 71-41-0 | 101 | 1.7028E+02 | -7.8640E+03 | -2.4335E+01 | 0 | 0 | 273.35 | 371.15 | < 10% | E |
| 1-HEXANOL | 111-27-3 | 101 | 1.7476E+02 | -7.6823E+03 | -2.4982E+01 | 0 | 0 | 298 | 363.15 | < 25% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-HEPTANOL | 111-70-6 | 101 | 2.0296E+02 | -8.6151E+03 | -2.9116E+01 | 0 | 0 | 273 | 375 | < 10% | EP |
| 1-OCTANOL | 111-87-5 | 101 | 3.4096E+02 | -1.5040E+04 | -4.9310E+01 | 0 | 0 | 288.15 | 363.45 | < 10% | EP |
| 1-NONANOL | 143-08-8 | 101 | 3.2991E+02 | -1.4056E+04 | -4.7688E+01 | 0 | 0 | 288.15 | 363.15 | < 25% | E |
| 1-DECANOL | 112-30-1 | 101 | 3.9199E+02 | -1.6451E+04 | -5.6942E+01 | 0 | 0 | 288.15 | 363.15 | < 10% | E |
| 1-UNDECANOL | 112-42-5 | 100 | 9.6801E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-DODECANOL | 112-53-8 | 100 | 3.9184E+06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| **N-ALIPHATIC PRIMARY AMINES** | | | | | | | | | | | |
| ETHYLAMINE | 75-04-7 | 100 | 4.7374E-01 | -1.1698E+04 | -3.3947E+01 | -9.1695E-03 | 1 | 298.15 | 298.15 | < 10% | S |
| n-PROPYLAMINE | 107-10-8 | 100 | 1.9970E+00 | -1.0633E+04 | -2.8801E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-BUTYLAMINE | 109-73-9 | 100 | 8.3162E+00 | -1.2774E+04 | -3.2890E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-PENTYLAMINE | 110-58-7 | 100 | 3.2117E+01 | -8.8828E+03 | -2.1253E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-HEXYLAMINE | 111-26-2 | 100 | 1.3205E+02 | 9.3895E+02 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-HEPTYLAMINE | 111-68-2 | 100 | 4.4889E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| n-OCTYLAMINE | 111-86-4 | 100 | 1.8558E+03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **N-ALKANES** | | | | | | | | | | | |
| n-PENTANE | 109-66-0 | 101 | -1.3467E+03 | 3.3236E+04 | 2.4123E+02 | -4.2847E-01 | 1 | 273.15 | 422.65 | < 25% | E |
| n-HEXANE | 110-54-3 | 101 | 3.6592E+02 | -1.6200E+04 | -5.2402E+01 | 0 | 0 | 273.15 | 443.15 | < 10% | E |
| n-HEPTANE | 142-82-5 | 101 | 3.7426E+02 | -1.6119E+04 | -5.3641E+01 | 0 | 0 | 273.15 | 443.75 | < 25% | E |
| n-OCTANE | 111-65-9 | 101 | 4.5088E+02 | -1.9596E+04 | -6.4794E+01 | 0 | 0 | 273.15 | 456.15 | < 25% | E |
| n-NONANE | 111-84-2 | 101 | 6.6057E+02 | -2.9453E+04 | -9.5478E+01 | 0 | 0 | 287.95 | 409.75 | < 50% | E |
| n-DECANE | 124-18-5 | 100 | 2.3009E+08 | -1.3625E+04 | -3.5395E+01 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **N-ALKYLBENZENES** | | | | | | | | | | | |
| BENZENE | 71-43-2 | 101 | 5.0455E+02 | -1.6685E+04 | -8.1666E+01 | 8.2232E-02 | 1 | 273.15 | 527.15 | < 3% | E |
| TOLUENE | 108-88-3 | 101 | 5.6897E+02 | -1.8250E+04 | -9.2692E+01 | 9.8716E-02 | 1 | 261.7 | 473.55 | < 5% | E |
| ETHYLBENZENE | 100-41-4 | 101 | 3.0277E+02 | -1.2921E+04 | -4.3705E+01 | 0 | 0 | 273.15 | 373.15 | < 5% | E |
| n-PROPYLBENZENE | 103-65-1 | 101 | 1.8059E+02 | -6.8317E+03 | -2.5610E+01 | 0 | 0 | 273.65 | 328.15 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-BUTYLBENZENE | 104-51-8 | 101 | 3.4172E+02 | -1.3779E+04 | -4.9545E+01 | 0 | 0 | 273.65 | 373.15 | < 5% | E |
| n-HEPTYLBENZENE | 1078-71-3 | 100 | 4.3293E+07 | -2.7892E+03 | 0 | 6.6631E+05 | -2 | 298.15 | 298.15 | < 10% | P |
| n-DECYLBENZENE | 104-72-3 | 100 | 4.8338E+09 | -6.0768E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| n-PENTYLBENZENE | 538-68-1 | 101 | 3.2086E+02 | -1.2951E+04 | -4.6121E+01 | 0 | 0 | 280.15 | 318.15 | < 10% | E |
| n-HEXYLBENZENE | 1077-16-3 | 101 | 2.8640E+02 | -1.1376E+04 | -4.0754E+01 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| n-OCTYLBENZENE | 2189-60-8 | 100 | 2.0136E+08 | -7.0790E+03 | -1.9442E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| n-NONYLBENZENE | 1081-77-2 | 100 | 9.6961E+08 | -8.8322E+02 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| **NAPHTHALENES** | | | | | | | | | | | |
| NAPHTHALENE | 91-20-3 | 101 | 2.7047E+02 | -1.0551E+04 | -3.9299E+01 | 0 | 0 | 275.05 | 346.55 | < 3% | E |
| 1-METHYLNAPHTHALENE | 90-12-0 | 101 | 8.4227E+00 | 1.2191E+03 | 0 | 0 | 0 | 277.25 | 304.85 | < 10% | E |
| 2-METHYLNAPHTHALENE | 91-57-6 | 101 | 7.1880E+00 | 1.6019E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| 1-ETHYLNAPHTHALENE | 1127-76-0 | 101 | 7.4549E+00 | 1.8432E+03 | 0 | 0 | 0 | 281.55 | 304.85 | < 10% | E |
| **NITRILES** | | | | | | | | | | | |
| ACETONITRILE | 75-05-8 | 101 | -3.4249E+01 | 1.3791E+03 | 5.5893E+00 | 0 | 0 | 273 | 353.15 | < 5% | E |
| PROPIONITRILE | 107-12-0 | 101 | 4.1879E+01 | -1.8363E+03 | -5.6957E+00 | 0 | 0 | 278.15 | 298.15 | < 25% | E |
| ACRYLONITRILE | 107-13-1 | 101 | 2.7998E+00 | 2.7737E+02 | 0 | 0 | 0 | 273.15 | 343.15 | < 3% | E |
| METHACRYLONITRILE | 126-98-7 | 101 | 2.3474E+02 | -1.0357E+04 | -3.4203E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | P |
| n-BUTYRONITRILE | 109-74-0 | 101 | 7.6172E+01 | -3.3874E+03 | -1.0547E+01 | 0 | 0 | 273.15 | 313.15 | < 3% | E |
| VALERONITRILE | 110-59-8 | 101 | 8.3220E+00 | -7.2378E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | E |
| ISOBUTYRONITRILE | 78-82-0 | 101 | 6.4645E+00 | -5.1172E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | E |
| BENZONITRILE | 100-47-0 | 101 | 2.6212E+02 | -1.0995E+04 | -3.8243E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| VINYLACETONITRILE | 109-75-1 | 101 | 4.8136E+00 | -3.2841E+01 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| PHENYLACETONITRILE | 140-29-4 | 101 | 7.9236E+00 | 1.1683E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 100% | E |
| **NITROAMINES** | | | | | | | | | | | |
| o-NITROANILINE | 88-74-4 | 101 | -2.5696E+00 | 3.1847E+03 | 0 | 0 | 0 | 298.15 | 313.25 | < 50% | E |
| p-NITROANILINE | 100-01-6 | 101 | -3.4304E+00 | 3.2308E+03 | 0 | 0 | 0 | 293.15 | 313.25 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **ORGANIC SALTS** | | | | | | | | | | | |
| DIETHYL CARBONATE | 105-58-8 | 101 | 1.8930E+02 | -8.8485E+03 | -2.6978E+01 | 0 | 0 | 273.15 | 363.45 | < 5% | E |
| DIMETHYL CARBONATE | 616-38-6 | 101 | 1.7097E+02 | -7.8524E+03 | -2.4703E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |
| **OTHER ALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| ISOPROPANOL | 67-63-0 | 101 | 1.4959E+02 | -7.7472E+03 | -2.1323E+01 | 0 | 0 | 273 | 373.15 | < 10% | E |
| 2-METHYL-1-PROPANOL | 78-83-1 | 101 | 2.7441E+02 | -1.2923E+04 | -3.9876E+01 | 0 | 0 | 273.35 | 374.15 | < 10% | E |
| 2-BUTANOL | 78-92-2 | 101 | 1.8600E+02 | -9.4446E+03 | -2.6519E+01 | 0 | 0 | 273 | 371.15 | < 5% | E |
| 2-METHYL-2-PROPANOL | 75-65-0 | 101 | 1.6764E+02 | -9.0892E+03 | -2.3636E+01 | 0 | 0 | 273 | 371.15 | < 10% | E |
| 2-PENTANOL | 6032-29-7 | 101 | 2.1732E+02 | -1.0616E+04 | -3.1087E+01 | 0 | 0 | 273.35 | 371.15 | < 5% | E |
| 2-METHYL-2-BUTANOL | 75-85-4 | 101 | 1.7560E+02 | -9.3077E+03 | -2.4714E+01 | 0 | 0 | 273.35 | 371.45 | < 5% | E |
| 2-METHYL-1-BUTANOL | 137-32-6 | 101 | 2.5881E+02 | -1.2308E+04 | -3.7301E+01 | 0 | 0 | 273.35 | 363.15 | < 5% | E |
| 2,2-DIMETHYL-1-PROPANOL | 75-84-3 | 101 | 2.2174E+02 | -1.1079E+04 | -3.1540E+01 | 0 | 0 | 285.15 | 363.15 | < 25% | P |
| 2-HEXANOL | 626-93-7 | 101 | 2.3127E+02 | -1.1094E+04 | -3.2981E+01 | 0 | 0 | 273.15 | 363.35 | < 25% | EP |
| 3-HEXANOL | 623-37-0 | 101 | 2.2426E+02 | -1.1042E+04 | -3.1824E+01 | 0 | 0 | 273.15 | 363.45 | < 5% | EP |
| 3-METHYL-1-PENTANOL | 589-35-5 | 101 | 2.4864E+02 | -1.1604E+04 | -3.5685E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | P |
| 3-METHYL-3-PENTANOL | 77-74-7 | 101 | 7.3413E+01 | -4.2766E+03 | -9.4714E+00 | 0 | 0 | 282.95 | 363.55 | < 10% | P |
| 3-PENTANOL | 584-02-1 | 101 | 2.1706E+02 | -1.0682E+04 | -3.1030E+01 | 0 | 0 | 273.35 | 371.15 | < 5% | E |
| 3-METHYL-1-BUTANOL | 123-51-3 | 101 | 3.5250E+02 | -1.6416E+04 | -5.1307E+01 | 0 | 0 | 273.35 | 374.15 | < 10% | E |
| 3-METHYL-2-BUTANOL | 598-75-4 | 101 | 2.1025E+02 | -1.0387E+04 | -3.0020E+01 | 0 | 0 | 273.35 | 371.15 | < 3% | E |
| 2-HEPTANOL | 543-49-7 | 101 | 2.5987E+02 | -1.2308E+04 | -3.7057E+01 | 0 | 0 | 273.15 | 363.35 | < 5% | P |
| 3-HEPTANOL | 589-82-2 | 101 | 2.2688E+02 | -1.1106E+04 | -3.2011E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | E |
| 4-METHYL-2-PENTANOL | 108-11-2 | 101 | 1.9584E+02 | -9.5636E+03 | -2.7711E+01 | 0 | 0 | 273.15 | 363.35 | < 10% | EP |
| 2-OCTANOL | 123-96-6 | 101 | 3.7853E+02 | -1.7786E+04 | -5.4429E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | P |
| 2-NONANOL | 628-99-9 | 101 | 3.8316E+02 | -1.8280E+04 | -5.4709E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | P |
| 2,6-DIMETHYL-4-HEPTANOL | 108-82-7 | 101 | 1.6061E+02 | -8.1347E+03 | -2.1735E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | P |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER ALIPHATIC AMINES** | | | | | | | | | | | |
| TRIETHYLAMINE | 121-44-8 | 100 | 6.5469E+01 | 6.5156E+03 | 2.1156E+01 | 8.2308E-06 | 2 | 298.15 | 298.15 | < 5% | S |
| DI-n-PROPYLAMINE | 142-84-7 | 100 | 7.1297E+01 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DIETHYLAMINE | 109-89-7 | 100 | 4.8211E+00 | 9.7708E+03 | 4.2873E+01 | -3.6254E-02 | 1 | 298.15 | 298.15 | < 25% | S |
| DI-n-BUTYLAMINE | 111-92-2 | 100 | 1.2008E+03 | 1.3625E+04 | 3.5395E+01 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| TRI-n-BUTYLAMINE | 102-82-9 | 101 | 1.3366E+01 | -1.1796E+03 | 0 | 0 | 0 | 273.15 | 353.15 | < 25% | E |
| **OTHER ALKANES** | | | | | | | | | | | |
| 2,3,4-TRIMETHYLPENTANE | 565-75-3 | 100 | 4.7045E+06 | 1.7539E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | P |
| 2,2,5-TRIMETHYLHEXANE | 3522-94-9 | 101 | 2.0543E+01 | -1.2384E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 10% | E |
| **OTHER ALKYLBENZENES** | | | | | | | | | | | |
| o-XYLENE | 95-47-6 | 101 | 2.6647E+02 | -1.0911E+04 | -3.8533E+01 | 0 | 0 | 273.15 | 353.15 | < 10% | E |
| m-XYLENE | 108-38-3 | 101 | 3.7934E+02 | -1.2942E+04 | 4.4713E-02 | -5.9466E+01 | 1 | 273.15 | 543.75 | < 10% | E |
| p-XYLENE | 106-42-3 | 101 | 7.1165E+02 | -2.4322E+04 | 1.0910E-01 | -1.1447E+02 | 1 | 273.15 | 568.05 | < 10% | E |
| CUMENE | 98-82-8 | 101 | 9.2874E+00 | 6.6679E+02 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| 1,2,3-TRIMETHYLBENZENE | 526-73-8 | 101 | 7.5122E+00 | 1.2115E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| 1,2,4-TRIMETHYLBENZENE | 95-63-6 | 101 | 8.2919E+00 | 1.0180E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 5% | E |
| MESITYLENE | 108-67-8 | 101 | 1.6957E+02 | -5.9219E+03 | -2.4197E+01 | 0 | 0 | 283.15 | 373.15 | < 25% | E |
| p-DIETHYLBENZENE | 105-05-5 | 100 | 2.9628E+05 | -5.1308E+03 | 0 | 0 | 0 | 293.15 | 293.15 | < 100% | E |
| 1,2,3,4-TETRAMETHYLBENZENE | 488-23-3 | 101 | 1.0233E+01 | 8.1540E+02 | 0 | 0 | 0 | 288.15 | 308.15 | < 100% | E |
| 1,2,4,5-TETRAMETHYLBENZENE | 95-93-2 | 100 | 6.0549E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| **OTHER AMINES, IMINES** | | | | | | | | | | | |
| CYCLOHEXYLAMINE | 108-91-8 | 101 | 1.4299E+02 | -8.3169E+03 | -1.9689E+01 | 0 | 0 | 298.15 | 372.82 | < 25% | E |
| TRIALLYLAMINE | 102-70-5 | 101 | 3.2999E+02 | -1.5808E+04 | -4.7217E+01 | 0 | 0 | 273.15 | 363.15 | < 25% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER CONDENSED RINGS** | | | | | | | | | | | |
| FLUORANTHENE | 206-44-0 | 101 | 4.0885E+00 | 3.6092E+03 | 0 | 0 | 0 | 281.25 | 333.15 | < 10% | E |
| FLUORENE | 86-73-7 | 101 | 3.8046E+00 | 3.0197E+03 | 0 | 0 | 0 | 279.75 | 333.15 | < 10% | E |
| ANTHRACENE | 120-12-7 | 101 | 2.8549E+02 | -2.0510E+04 | -3.8180E+01 | 0 | 0 | 273.45 | 347.85 | < 5% | E |
| PHENANTHRENE | 85-01-8 | 101 | 2.4635E+02 | -7.8027E+03 | -3.6051E+01 | 0 | 0 | 277.15 | 346.55 | < 5% | E |
| CHRYSENE | 218-01-9 | 101 | 1.0112E+01 | 2.7117E+03 | 0 | 0 | 0 | 279.65 | 302.15 | < 25% | E |
| PYRENE | 129-00-0 | 101 | 2.8752E+02 | -9.6725E+03 | -4.1927E+01 | 0 | 0 | 277.85 | 347.85 | < 5% | E |
| ACENAPHTHENE | 83-32-9 | 101 | 4.2310E+00 | 2.6602E+03 | 0 | 0 | 0 | 277.25 | 347.85 | < 25% | E |
| ACENAPHTHALENE | 208-96-8 | 101 | 6.4639E+00 | 1.9187E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| BENZO[a]PYRENE | 50-32-8 | 101 | 7.4109E+00 | 4.1135E+03 | 0 | 0 | 0 | 281.15 | 308.15 | < 10% | E |
| BENZO[b]FLUORANTHENE | 205-99-2 | 101 | -2.0161E+00 | 6.3942E+03 | 0 | 0 | 0 | 283.15 | 328.15 | < 10% | E |
| **OTHER ETHERS/DIETHERS** | | | | | | | | | | | |
| METHYLAL | 109-87-5 | 101 | 6.6045E+00 | -1.1224E+03 | 0 | 0 | 0 | 273.35 | 333.15 | < 25% | E |
| 1,2-DIMETHOXYETHANE | 110-71-4 | 101 | 1.9979E+02 | -1.1271E+04 | -2.8177E+01 | 0 | 0 | 273.35 | 372.5 | < 3% | E |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 112-73-2 | 101 | 2.5849E+01 | -5.0993E+03 | 0 | 0 | 0 | 273.15 | 293.15 | < 100% | P |
| ANISOLE | 100-66-3 | 101 | 3.7640E+00 | 1.3538E+03 | 0 | 0 | 0 | 275.15 | 363.85 | < 5% | E |
| DIPHENYL ETHER | 101-84-8 | 100 | 4.9071E+05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **OTHER INORGANICS** | | | | | | | | | | | |
| HYDROGEN PEROXIDE | 7722-84-1 | 101 | 1.1957E+00 | -8.0509E+02 | 0 | 0 | 0 | 278.15 | 297.15 | < 25% | E |
| **OTHER MONOAROMATICS** | | | | | | | | | | | |
| STYRENE | 100-42-5 | 101 | 4.1793E+00 | 1.6920E+03 | 0 | 0 | 0 | 293.32 | 313.02 | < 5% | E |
| **OTHER POLYFUNCTIONAL C, H, O** | | | | | | | | | | | |
| 2-BUTOXYETHANOL | 111-76-2 | 101 | 8.7199E+00 | -1.5162E+03 | 0 | 0 | 0 | 293.15 | 303.15 | < 25% | E |
| VANILLIN | 121-33-5 | 101 | -4.5897E+02 | 2.2705E+04 | 6.8209E+01 | 0 | 0 | 293.15 | 318.15 | < 5% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER POLYFUNCTIONAL ORGANICS** | | | | | | | | | | | |
| MALATHION | 121-75-5 | 101 | 9.4811E+00 | 6.5738E+02 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| **OTHER SATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ISOVALERATE | 108-64-5 | 101 | 1.9687E+02 | -9.4132E+03 | -2.7576E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| DIETHYL MALONATE | 105-53-3 | 101 | 2.1777E+02 | -1.0033E+04 | -3.1264E+01 | 0 | 0 | 273.15 | 363.75 | < 10% | P |
| ETHYL TRIMETHYL ACETATE | 3938-95-2 | 101 | 1.7393E+02 | -8.6446E+03 | -2.3987E+01 | 0 | 0 | 273.15 | 363.55 | < 25% | E |
| **PEROXIDES** | | | | | | | | | | | |
| METHYL HYDROPEROXIDE | 3031-73-0 | 101 | 1.0534E+00 | 7.9863E+01 | 0 | 0 | 0 | 277.15 | 297.15 | < 3% | E |
| ETHYL HYDROPEROXIDE | 3031-74-1 | 101 | 2.7406E+00 | -3.6257E+02 | 0 | 0 | 0 | 278.15 | 297.15 | < 10% | E |
| **POLYFUNCTIONAL AMIDES/AMINES** | | | | | | | | | | | |
| N,N-DIMETHYLFORMAMIDE | 68-12-2 | 101 | 1.4648E+02 | -8.3423E+03 | -2.0868E+01 | 0 | 0 | 289.4 | 372 | < 25% | E |
| N-METHYLFORMAMIDE | 123-39-7 | 101 | 2.0381E+00 | -5.8045E+02 | 0 | 0 | 0 | 333.15 | 372.65 | < 5% | E |
| N,N-DIMETHYLACETAMIDE | 127-19-5 | 101 | 7.5170E+00 | -2.4924E+03 | 0 | 0 | 0 | 343.15 | 372.28 | < 10% | E |
| **POLYFUNCTIONAL C, H, N, HALIDE, (O)** | | | | | | | | | | | |
| o-CHLOROANILINE | 95-51-2 | 101 | 1.2561E+03 | -4.1122E+04 | -2.0798E+02 | 2.4659E-01 | 1 | 298.15 | 431.15 | < 25% | P |
| p-CHLORONITROBENZENE | 100-00-5 | 101 | 2.1438E+00 | 2.3385E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| **POLYFUNCTIONAL C, H, O, HALIDE** | | | | | | | | | | | |
| DI(2-CHLOROETHYL)ETHER | 111-44-4 | 101 | 1.5144E+02 | -6.4595E+03 | -2.1611E+01 | 0 | 0 | 273.15 | 364.85 | < 5% | E |
| ETHYLCHLOROACETATE | 105-39-5 | 101 | 1.9772E+02 | -8.9873E+03 | -2.8391E+01 | 0 | 0 | 273.15 | 333.25 | < 10% | E |
| METHYL CHLOROACETATE | 96-34-4 | 101 | 1.0528E+02 | -4.4693E+03 | -1.5019E+01 | 0 | 0 | 273.15 | 323.35 | < 5% | E |
| **POLYFUNCTIONAL C, H, O, N** | | | | | | | | | | | |
| N-METHYL-2-PYRROLIDONE | 872-50-4 | 101 | 3.9967E+02 | -2.1700E+04 | -5.7549E+01 | 0 | 0 | 298.8 | 372.85 | < 5% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **POLYFUNCTIONAL C, H, O, S** | | | | | | | | | | | |
| DIMETHYL SULFOXIDE | 67-68-5 | 101 | 2.9405E+00 | -1.6085E+03 | 0 | 0 | 0 | 298.8 | 337.9 | < 25% | E |
| **POLYFUNCTIONAL ESTERS** | | | | | | | | | | | |
| METHYL SALICYLATE | 119-36-8 | 101 | 1.6195E+02 | -6.2843E+03 | -2.3185E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| 2-ETHOXYETHYL ACETATE | 111-15-9 | 100 | 4.7700E+01 | 0 | 0 | 0 | 0 | 303.15 | 303.15 | < 10% | E |
| ETHYL ACETOACETATE | 141-97-9 | 101 | 6.4902E+00 | -6.8868E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | EP |
| ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 112-07-2 | 100 | 2.6459E+02 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| **PROPIONATES AND BUTYRATES** | | | | | | | | | | | |
| METHYL PROPIONATE | 554-12-1 | 101 | 8.7616E+00 | -1.2878E+03 | 0 | 0 | 0 | 273.15 | 310.2 | < 5% | E |
| ETHYL PROPIONATE | 105-37-3 | 101 | 2.3017E+02 | -1.0936E+04 | -3.2963E+01 | 0 | 0 | 273.15 | 353.45 | < 25% | E |
| n-PROPYL PROPIONATE | 106-36-5 | 101 | 1.7662E+02 | -8.7139E+03 | -2.4641E+01 | 0 | 0 | 273.15 | 363.65 | < 10% | E |
| n-BUTYL PROPIONATE | 590-01-2 | 101 | 2.1594E+02 | -1.0309E+04 | -3.0373E+01 | 0 | 0 | 273.15 | 363.55 | < 10% | E |
| n-PROPYL n-BUTYRATE | 105-66-8 | 101 | 2.0811E+02 | -9.7622E+03 | -2.9327E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| METHYL n-BUTYRATE | 623-42-7 | 101 | 1.0572E+02 | -5.2463E+03 | -1.4460E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ETHYL n-BUTYRATE | 105-54-4 | 101 | 1.4646E+02 | -7.2997E+03 | -2.0200E+01 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ISOBUTYL ISOBUTYRATE | 97-85-8 | 101 | 2.2011E+02 | -1.0408E+04 | -3.0834E+01 | 0 | 0 | 273.15 | 363.45 | < 25% | E |
| n-BUTYL n-BUTYRATE | 109-21-7 | 101 | 2.9628E+02 | -1.4154E+04 | -4.2014E+01 | 0 | 0 | 273.15 | 363.45 | < 10% | E |
| METHYL ISOBUTYRATE | 547-63-7 | 101 | 1.4441E+02 | -7.0836E+03 | -2.0168E+01 | 0 | 0 | 273.15 | 353.45 | < 10% | E |
| ETHYL ISOBUTYRATE | 97-62-1 | 101 | 1.4146E+02 | -7.0790E+03 | -1.9442E+01 | 0 | 0 | 273.15 | 363.75 | < 10% | P |
| n-PENTYL n-BUTYRATE | 540-18-1 | 101 | 1.1097E+01 | -2.1866E+02 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ISOPENTYL BUTYRATE | 106-27-4 | 101 | 2.4293E+02 | -1.1495E+04 | -3.4028E+01 | 0 | 0 | 282.55 | 363.85 | < 100% | E |
| **SULFIDES/THIOPHENES** | | | | | | | | | | | |
| DIMETHYL SULFIDE | 75-18-3 | 101 | 1.6724E+02 | -7.3055E+03 | -2.4157E+01 | 0 | 0 | 272.35 | 353.45 | < 10% | E |
| DIMETHYL DISULFIDE | 624-92-0 | 101 | 4.5046E+00 | 8.8438E+02 | 0 | 0 | 0 | 273.2 | 343.15 | < 10% | E |

Table C.3: $\gamma_i^\infty$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-METHYLTHIOPHENE | 554-14-3 | 101 | 7.2541E+00 | 3.1691E+02 | 0 | 0 | 0 | 298.15 | 343.15 | < 10% | E |
| DIISOPROPYL SULFIDE | 625-80-9 | 101 | 9.7925E+00 | -2.6053E+02 | 0 | 0 | 0 | 298.15 | 343.15 | < 10% | E |
| **UNSATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ACRYLATE | 140-88-5 | 101 | 5.2318E+00 | 1.1910E+02 | 0 | 0 | 0 | 298.6 | 360.2 | < 10% | P |
| METHYL METHACRYLATE | 80-62-6 | 101 | 2.1314E+02 | -9.7326E+03 | -3.0636E+01 | 0 | 0 | 273.35 | 333.15 | < 3% | E |

Table C.4: $x_i^{aq}$ regression summary

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **1-ALKENES** | | | | | | | | | | | |
| 1-PENTENE | 109-67-1 | 100 | 4.5386E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXENE | 592-41-6 | 100 | 1.0983E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-HEPTENE | 592-76-7 | 100 | 2.6578E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-OCTENE | 111-66-0 | 100 | 6.4314E-07 | -1.2631E+04 | -3.2632E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| 1-NONENE | 124-11-8 | 100 | 1.5564E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-DECENE | 872-05-9 | 100 | 3.7663E-08 | -2.1023E+04 | -4.4514E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-UNDECENE | 872-05-9 | 100 | 9.1136E-09 | -1.9152E+04 | -3.3127E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-DODECENE | 872-05-9 | 100 | 2.2055E-09 | -8.1347E+03 | -2.1735E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-TRIDECENE | 592-41-6 | 100 | 5.3369E-10 | 1.6356E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| 1-TETRADECENE | 872-05-9 | 100 | 1.2916E-10 | -1.8992E+04 | -3.6878E+01 | 0 | 0 | 298.15 | 298.15 | < 50% | P |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-PENTADECENE | 13360-61-7 | 100 | 3.1253E-11 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **2,3,4-ALKENES** | | | | | | | | | | | |
| cis-2-PENTENE | 627-20-3 | 100 | 5.2143E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| trans-2-PENTENE | 646-04-8 | 100 | 5.2143E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| cis-2-HEPTENE | 6443-92-1 | 100 | 2.7522E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| trans-2-HEPTENE | 14686-13-6 | 100 | 2.7522E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| **ACETATES** | | | | | | | | | | | |
| METHYL ACETATE | 79-20-9 | 101 | -2.3084E+03 | 1.9554E+05 | 3.1910E+02 | -1.4952E+07 | -2 | 278.15 | 356.65 | < 3% | E |
| ETHYL ACETATE | 141-78-6 | 101 | -1.3361E+03 | 1.0978E+05 | 1.8495E+02 | -7.9991E+06 | -2 | 273.15 | 343.65 | < 3% | E |
| n-PROPYL ACETATE | 109-60-4 | 101 | 4.8913E+00 | -7.2626E+03 | 0 | 1.2351E+06 | -2 | 273.15 | 363.35 | < 5% | E |
| n-BUTYL ACETATE | 123-86-4 | 101 | 3.1799E+00 | -6.9848E+03 | 0 | 1.1870E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| ISOBUTYL ACETATE | 110-19-0 | 101 | 8.7151E+00 | -1.0152E+04 | 0 | 1.6438E+06 | -2 | 273.15 | 420.25 | < 10% | E |
| ISOPENTYL ACETATE | 123-92-2 | 101 | 6.9823E+00 | -1.0058E+04 | 0 | 1.6541E+06 | -2 | 273.15 | 363.85 | < 10% | E |
| ISOPROPYL ACETATE | 108-21-4 | 101 | 6.2087E+00 | -8.1630E+03 | 0 | 1.4057E+06 | -2 | 273.15 | 366.15 | < 10% | E |
| sec-BUTYL ACETATE | 105-46-4 | 101 | 3.8824E+00 | -7.4666E+03 | 0 | 1.2842E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| VINYL ACETATE | 108-05-4 | 101 | 3.3355E+00 | -5.4481E+03 | 0 | 8.6465E+05 | -2 | 273.35 | 333.15 | < 3% | E |
| n-PENTYL ACETATE | 628-63-7 | 101 | 1.3007E+01 | -1.4017E+04 | 0 | 2.2856E+06 | -2 | 273.15 | 364.5 | < 25% | E |
| n-HEXYL ACETATE | 142-92-7 | 101 | 1.7463E+01 | -1.7134E+04 | 0 | 2.6915E+06 | -2 | 273.15 | 363.35 | < 25% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-HEPTYL ACETATE | 112-06-1 | 100 | 1.5184E-05 | -1.5368E+04 | -3.7557E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| n-OCTYL ACETATE | 112-14-1 | 100 | 3.7799E-06 | -1.1079E+04 | -3.1540E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| ETHYLENE GLYCOL DIACETATE | 111-55-7 | 101 | 6.4818E+00 | -6.0277E+03 | 0 | 8.8752E+05 | -2 | 273.15 | 363.25 | < 3% | E |
| tert-BUTYL ACETATE | 540-88-5 | 101 | 1.3823E+00 | -6.1464E+03 | 0 | 1.1073E+06 | -2 | 273.15 | 353.65 | < 3% | E |
| CYCLOHEXYL ACETATE | 622-45-7 | 101 | 4.5951E+00 | -8.3650E+03 | 0 | 1.3772E+06 | -2 | 273.15 | 363.45 | < 10% | E |
| PHENYL ACETATE | 122-79-2 | 101 | 6.0837E+00 | -7.8765E+03 | 0 | 1.1694E+06 | -2 | 273.15 | 363.95 | < 10% | E |
| **ALDEHYDES** | | | | | | | | | | | |
| ACETALDEHYDE | 75-07-0 | 101 | -2.0000E+01 | 5.5703E+03 | 0 | 0 | 0 | 294.15 | 318.15 | < 10% | P |
| PROPANAL | 123-38-6 | 101 | -1.0158E+01 | 2.4071E+03 | 0 | 0 | 0 | 285.45 | 323.15 | < 25% | E |
| BUTANAL | 123-72-8 | 101 | -9.0064E+00 | 1.4733E+03 | 0 | 0 | 0 | 273.15 | 343.15 | < 10% | E |
| 2-METHYLPROPANAL | 78-84-2 | 101 | -8.9679E+00 | 1.3843E+03 | 0 | 0 | 0 | 273.15 | 333.15 | < 5% | E |
| PENTANAL | 110-62-3 | 101 | -9.8645E+00 | 1.2720E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 50% | E |
| HEPTANAL | 111-71-7 | 101 | 1.5461E+01 | -1.5603E+04 | 0 | 2.5355E+06 | -2 | 273.15 | 363.15 | < 10% | E |
| HEXANAL | 66-25-1 | 101 | 1.7602E+01 | -1.6591E+04 | 0 | 2.7535E+06 | -2 | 273.15 | 373.15 | < 25% | E |
| OCTANAL | 124-13-0 | 101 | -1.3858E+01 | 1.2453E+03 | 0 | 0 | 0 | 283.15 | 318.15 | < 50% | E |
| NONANAL | 124-19-6 | 101 | -8.9336E+00 | -8.6592E+02 | 0 | 0 | 0 | 283.15 | 318.15 | < 50% | E |
| 2-ETHYLHEXANAL | 123-05-7 | 101 | -8.2417E+00 | -4.5642E+02 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-ETHYL-2-HEXENAL | 645-62-5 | 101 | -8.3157E+00 | -1.0075E+02 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| DECANAL | 112-31-2 | 101 | -1.6848E+01 | 1.0170E+03 | 0 | 0 | 0 | 298.15 | 318.15 | < 50% | E |
| 2-METHYL-BUTYRALDEHYDE | 96-17-3 | 101 | -9.8239E+00 | 1.2190E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| ACROLEIN | 107-02-8 | 5000 | -1.0495E+04 | 6.6687E+04 | 1.5256E+03 | 1.3239E+03 | 361.35 | 273.15 | 361.15 | < 10% | E |
| trans-CROTONALDEHYDE | 123-73-9 | 101 | 4.1230E+00 | -4.8483E+03 | 0 | 8.0558E+05 | -2 | 273.15 | 363.15 | < 10% | E |
| METHACROLEIN | 78-85-3 | 101 | -6.5100E+00 | 7.1224E+02 | 0 | 0 | 0 | 273.15 | 333.15 | < 10% | E |
| p-TOLUALDEHYDE | 104-87-0 | 101 | -5.9618E+00 | -6.6380E+02 | 0 | 0 | 0 | 273.15 | 363.15 | < 10% | E |
| BENZALDEHYDE | 100-52-7 | 101 | 1.1413E+01 | -1.0321E+04 | 0 | 1.4635E+06 | -2 | 273.08 | 373.15 | < 10% | E |
| **ALIPHATIC ETHERS** | | | | | | | | | | | |
| DIETHYL ETHER | 60-29-7 | 101 | -1.2269E+01 | 2.4068E+03 | 0 | 0 | 0 | 269.32 | 307.25 | < 5% | E |
| DIISOPROPYL ETHER | 108-20-3 | 101 | -1.9779E+01 | 5.2627E+03 | 0 | -3.8263E+05 | -2 | 273.15 | 334.15 | < 10% | E |
| DI-n-BUTYL ETHER | 142-96-1 | 101 | -1.5032E+01 | 1.3926E+03 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| METHYL tert-BUTYL ETHER | 1634-04-4 | 101 | -8.9827E+00 | 2.3199E+02 | 0 | 3.0025E+05 | -2 | 273.15 | 343.15 | < 10% | E |
| METHYL ISOBUTYL ETHER | 625-44-5 | 101 | -1.5502E+01 | 2.8024E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 5% | E |
| DI-n-HEXYL ETHER | 112-58-3 | 100 | 6.8917E-08 | -3.2876E+04 | -7.4441E+01 | 0 | 0 | 298.15 | 298.15 | < 25% | P |
| METHYL n-BUTYL ETHER | 628-28-4 | 101 | -1.8085E+01 | 3.4942E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 25% | E |
| DI-n-PENTYL ETHER | 693-65-2 | 100 | 2.2173E-06 | -1.2187E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| METHYL tert-PENTYL ETHER | 994-05-8 | 101 | -1.4359E+00 | -5.3257E+03 | 0 | 1.1530E+06 | -2 | 273.15 | 352.35 | < 10% | E |
| tert-BUTYL ETHYL ETHER | 637-92-3 | 101 | -1.5992E+01 | 2.9990E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| ETHYL tert-PENTYL ETHER | 919-94-8 | 101 | -1.7642E+01 | 2.9896E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| DI-n-PROPYL ETHER | 111-43-3 | 101 | 1.4439E+01 | -1.5271E+04 | 0 | 2.5850E+06 | -2 | 273.15 | 333.25 | < 10% | E |
| n-BUTYL ETHYL ETHER | 628-81-9 | 101 | 5.5361E+00 | -8.7602E+03 | 0 | 1.5059E+06 | -2 | 273.15 | 363.85 | < 25% | E |
| **ALKYLCYCLOHEXANES** | | | | | | | | | | | |
| METHYL-CYCLOHEXANE | 108-87-2 | 101 | 2.2613E+01 | -2.1770E+04 | 0 | 3.3465E+06 | -2 | 293.15 | 443.95 | < 25% | E |
| ETHYL-CYCLOHEXANE | 1678-91-7 | 101 | 5.7107E+02 | -6.9022E+04 | -7.5554E+01 | 6.8089E+06 | -2 | 274.15 | 443.95 | < 10% | E |
| cis-1,2-DIMETHYL-CYCLOHEXANE | 2207-01-4 | 101 | 9.2417E+00 | -1.3497E+04 | 0 | 1.9708E+06 | -2 | 274.15 | 313.15 | < 3% | E |
| trans-1,2-DIMETHYL-CYCLOHEXANE | 6876-23-9 | 101 | 4.0532E+02 | -5.4401E+04 | -5.2782E+01 | 5.6689E+06 | -2 | 274.15 | 443.25 | < 5% | E |
| ALKYL-CYCLOPENTANES | | | | | | | | | | | |
| METHYL-CYCLOPENTANE | 96-37-7 | 100 | 9.1506E-06 | -1.3517E+04 | -3.1894E+01 | 0 | 0 | 298.15 | 298.15 | < 3% | S |
| **ALKYNES** | | | | | | | | | | | |
| ETHYLACETYLENE | 107-00-6 | 100 | 1.0280E-03 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-PENTYNE | 627-19-0 | 100 | 4.0450E-04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-HEXYNE | 693-02-7 | 100 | 8.4660E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-OCTYNE | 629-05-0 | 100 | 3.9470E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-NONYNE | 3452-09-3 | 100 | 7.6320E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-HEPTYNE | 628-71-7 | 100 | 1.8240E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| **AROMATIC ALCOHOLS** | | | | | | | | | | | |
| 2,3-XYLENOL | 526-75-0 | 6000 | -1.5683E+01 | 1.6800E+03 | 2.0352E-02 | -4.5266E+00 | 483.26 | 293.15 | 483.25 | < 25% | E |
| 2,4-XYLENOL | 105-67-9 | 6000 | -2.3457E+01 | 3.2524E+03 | 2.8887E-02 | -3.8002E+00 | 486.06 | 298.15 | 486.05 | < 25% | E |
| 2,5-XYLENOL | 95-87-4 | 6000 | 1.1654E+01 | -3.1846E+03 | -1.4892E-02 | -5.5852E+00 | 492.16 | 293.15 | 492.15 | < 25% | E |
| 2,6-XYLENOL | 576-26-1 | 6000 | -2.9019E+01 | 4.1106E+03 | 3.6790E-02 | -3.6459E+00 | 514.35 | 293.15 | 514.35 | < 25% | E |
| 3,4-XYLENOL | 95-65-8 | 6000 | -1.4145E+00 | -4.9478E+02 | 1.1971E-04 | -5.6703E+00 | 463.36 | 293.15 | 463.35 | < 25% | E |
| 3,5-XYLENOL | 108-68-9 | 6000 | 3.1997E+00 | -1.1427E+03 | -6.1815E-03 | -6.5122E+00 | 473.16 | 293.15 | 473.15 | < 25% | E |
| BENZYL ALCOHOL | 100-51-6 | 6000 | -1.7550E+01 | 2.6630E+03 | 2.1755E-02 | -4.1474E+00 | 421.66 | 273.15 | 421.65 | < 10% | E |
| PHENOL | 108-95-2 | 6000 | -2.6083E+01 | 4.1611E+03 | 3.5914E-02 | -5.3947E+00 | 341.46 | 273.15 | 341.45 | < 10% | E |
| o-CRESOL | 95-48-7 | 6000 | -5.1769E+00 | 6.8531E+02 | 4.0436E-03 | -5.4711E+00 | 439.66 | 273.15 | 439.65 | < 25% | E |
| m-CRESOL | 108-39-4 | 6000 | -6.2483E+00 | 8.1278E+02 | 5.3851E-03 | -5.4723E+00 | 421.86 | 272.95 | 421.85 | < 10% | E |
| p-CRESOL | 106-44-5 | 6000 | 1.3914E+01 | -2.4840E+03 | -2.4577E-02 | -6.0623E+00 | 416.86 | 273.15 | 416.85 | < 10% | E |
| p-ETHYLPHENOL | 123-07-9 | 6000 | -9.4585E+00 | 1.6912E+03 | 7.9368E-03 | -7.7616E+00 | 460.26 | 298.15 | 460.25 | < 50% | E |
| 2-PHENYLETHANOL | 60-12-8 | 101 | 1.0118E+01 | -9.3144E+03 | 0 | 1.3785E+06 | -2 | 283.15 | 373.15 | < 10% | E |
| 1-PHENYL-1-PROPANOL | 93-54-9 | 101 | 8.8268E+00 | -9.9590E+03 | 0 | 1.5984E+06 | -2 | 293.15 | 363.65 | < 5% | E |
| **AROMATIC AMINES** | | | | | | | | | | | |
| o-TOLUIDINE | 95-53-4 | 101 | -5.6696E+00 | -4.1271E+01 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| m-TOLUIDINE | 108-44-1 | 101 | -5.6334E+00 | -9.0608E+01 | 0 | 0 | 0 | 298.15 | 323.15 | < 25% | E |
| p-TOLUIDINE | 106-49-0 | 101 | 6.4902E+00 | -3.8937E+03 | 0 | 0 | 0 | 293.15 | 313.15 | < 5% | E |
| QUINOLINE | 91-22-5 | 101 | -6.5531E+02 | 5.0239E+04 | 9.1044E+01 | -3.4520E+06 | -2 | 273.15 | 498.2 | < 25% | E |
| N,N-DIETHYLANILINE | 91-66-7 | 101 | -9.3555E+00 | -4.0851E+02 | 0 | 0 | 0 | 273.15 | 333.15 | < 10% | E |
| PYRIDINE | 110-86-1 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 368.15 | U | E |
| ANILINE | 62-53-3 | 101 | 7.6638E+00 | -7.1200E+03 | 0 | 1.0031E+06 | -2 | 281.75 | 369.85 | < 3% | E |
| 2-METHYLPYRIDINE | 109-06-8 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 368.15 | U | E |
| o-ETHYLANILINE | 578-54-1 | 101 | 5.2059E+00 | -7.4833E+03 | 0 | 1.1569E+06 | -2 | 283.15 | 363.15 | < 10% | E |
| 2,4,6-TRIMETHYL-PYRIDINE | 108-75-8 | 6000 | -2.4933E+01 | 3.0991E+03 | 3.6399E-02 | -4.2595E+00 | 279.64 | 279.65 | 363.15 | < 25% | E |
| 2,6-DIMETHYL-PYRIDINE | 108-48-5 | 6000 | -5.0882E+01 | 7.5209E+03 | 7.6927E-02 | -4.9826E+00 | 307.14 | 307.15 | 363.15 | < 10% | E |
| 3-METHYLPYRIDINE | 108-99-6 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 368.15 | U | E |
| 4-METHYL-PYRIDINE | 108-89-4 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 368.15 | U | E |
| 2,4-DIMETHYL-ANILINE | 95-68-1 | 101 | 1.2321E+01 | -1.2131E+04 | 0 | 1.8891E+06 | -2 | 273.15 | 363.15 | < 10% | E |
| N-ETHYLANILINE | 103-69-5 | 101 | 7.1042E+00 | -9.4288E+03 | 0 | 1.4841E+06 | -2 | 273.15 | 363.15 | < 5% | E |
| **AROMATIC CARBOXYLIC ACIDS** | | | | | | | | | | | |
| o-TOLUIC ACID | 118-90-1 | 6000 | 1.5306E+00 | -2.9748E+03 | 6.5706E-03 | -3.3513E+00 | 434.36 | 278.15 | 434.35 | < 25% | E |
| p-TOLUIC ACID | 99-94-5 | 101 | 2.0163E+01 | -1.4966E+04 | 0 | 1.7837E+06 | -2 | 278.15 | 343.15 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PHTHALIC ACID | 88-99-3 | 101 | -3.2559E+03 | 2.8099E+05 | 4.4935E+02 | -2.2581E+07 | -2 | 283.65 | 352.45 | < 5% | E |
| m-TOLUIC ACID | 99-04-7 | 101 | 2.4555E+01 | -1.6880E+04 | 0 | 2.0431E+06 | -2 | 278.15 | 348.15 | < 3% | E |
| **AROMATIC CHLORIDES** | | | | | | | | | | | |
| BENZYL CHLORIDE | 100-44-7 | 101 | -4.8047E+00 | -1.4232E+03 | 0 | 0 | 0 | 277.65 | 303.15 | < 25% | E |
| MONO-CHLOROBENZENE | 108-90-7 | 101 | 1.9378E+01 | -1.6010E+04 | 0 | 2.2051E+06 | -2 | 274.15 | 353.16 | < 10% | E |
| o-DICHLOROBENZENE | 95-50-1 | 101 | 4.6100E+01 | -3.3265E+04 | 0 | 4.8466E+06 | -2 | 278.15 | 318.15 | < 10% | E |
| m-DICHLOROBENZENE | 541-73-1 | 101 | -7.2884E+00 | -1.1202E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 10% | E |
| p-DICHLOROBENZENE | 106-46-7 | 101 | 1.9920E+01 | -1.6897E+04 | 0 | 2.2424E+06 | -2 | 278.15 | 346.55 | < 10% | E |
| HEXACHLORO-BENZENE | 118-74-1 | 101 | -8.8149E+00 | -3.8499E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| o-CHLOROTOLUENE | 95-49-8 | 101 | -7.5182E+00 | -1.0005E+03 | 0 | 0 | 0 | 274.15 | 318.15 | < 25% | E |
| p-CHLOROTOLUENE | 106-43-4 | 101 | -7.6410E+00 | -9.8024E+02 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 2,4-DICHLOROTOLUENE | 95-73-8 | 101 | -8.0197E+00 | -1.4022E+03 | 0 | 0 | 0 | 278.15 | 323.1 | < 10% | E |
| 1,2,4-TRICHLORO-BENZENE | 120-82-1 | 101 | -7.9726E+00 | -1.3232E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| 1,2,3-TRICHLORO-BENZENE | 87-61-6 | 101 | -1.3063E+00 | -3.5211E+03 | 0 | 0 | 0 | 277.15 | 323.15 | < 25% | E |
| **AROMATIC ESTERS** | | | | | | | | | | | |
| BENZYL ACETATE | 140-11-4 | 101 | 4.7216E+00 | -7.2941E+03 | 0 | 1.0365E+06 | -2 | 273.15 | 363.55 | < 10% | E |
| DI-n-PROPYL PHTHALATE | 131-16-8 | 100 | 6.6314E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| DI-n-HEXYL PHTHALATE | 84-75-3 | 100 | 1.2643E-08 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| METHYL BENZOATE | 93-58-3 | 101 | 8.7933E+00 | -9.7990E+03 | 0 | 1.4112E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| ETHYL BENZOATE | 93-89-0 | 101 | 2.7651E+00 | -7.0158E+03 | 0 | 1.0392E+06 | -2 | 273.15 | 363.45 | < 25% | E |
| BENZYL FORMATE | 104-57-4 | 101 | 2.3594E+01 | -1.8379E+04 | 0 | 2.7903E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| DIETHYL PHTHALATE | 84-66-2 | 101 | -3.2340E-01 | -5.6461E+03 | 0 | 8.6853E+05 | -2 | 278.15 | 323.15 | < 10% | E |
| DI-n-BUTYL PHTHALATE | 84-74-2 | 101 | 4.3454E+01 | -3.4620E+04 | 0 | 5.1921E+06 | -2 | 283.15 | 323.15 | < 25% | E |
| DIMETHYL PHTHALATE | 131-11-3 | 101 | 7.9570E+00 | -8.8956E+03 | 0 | 1.2524E+06 | -2 | 283.15 | 323.15 | < 5% | E |
| **C, H, BR COMPOUNDS** | | | | | | | | | | | |
| BROMOMETHANE | 74-83-9 | 101 | -1.7476E+01 | 3.4457E+03 | 0 | 0 | 0 | 273.15 | 305.15 | < 25% | E |
| BROMOETHANE | 74-96-4 | 101 | -8.0017E+00 | 4.4804E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 3% | E |
| 1,1,2,2-TETRABROMO-ETHANE | 79-27-6 | 101 | 6.9918E+00 | -6.0683E+03 | 0 | 0 | 0 | 298.15 | 323.15 | < 50% | E |
| 1-BROMOPROPANE | 106-94-5 | 101 | -1.0015E+01 | 6.1560E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| 2-BROMOPROPANE | 75-26-3 | 101 | 1.4812E+01 | -1.3646E+04 | 0 | 2.0705E+06 | -2 | 273.15 | 303.15 | < 5% | E |
| 1-BROMOBUTANE | 109-65-9 | 100 | 7.4063E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1-BROMOHEPTANE | 629-04-9 | 100 | 7.4417E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 1,2-DIBROMOETHANE | 106-93-4 | 101 | -5.9500E+00 | -5.3923E+02 | 0 | 0 | 0 | 273.15 | 363.75 | < 10% | E |
| m-DIBROMOBENZENE | 108-36-1 | 100 | 7.5328E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | E |
| BROMOBENZENE | 108-86-1 | 101 | 2.4459E+01 | -1.9666E+04 | 0 | 2.8011E+06 | -2 | 283.15 | 343.15 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| TRIBROMO-METHANE | 75-25-2 | 101 | -6.7179E+00 | -4.8067E+02 | 0 | 0 | 0 | 283 | 313.15 | < 10% | E |
| DIBROMO-METHANE | 74-95-3 | 101 | -9.0240E-01 | -3.2490E+03 | 0 | 4.5394E+05 | -2 | 273.15 | 363.25 | < 5% | E |
| 2-BROMOBUTANE | 78-76-2 | 100 | 1.2019E-04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| p-BROMOTOLUENE | 106-38-7 | 101 | -7.8116E+00 | -1.0704E+03 | 0 | 0 | 0 | 293.1 | 322.91 | < 25% | E |
| **C, H, F COMPOUNDS** | | | | | | | | | | | |
| METHYL FLUORIDE | 593-53-3 | 101 | -4.3912E+00 | -3.6301E+03 | 0.0000E+00 | 8.6381E+05 | -2 | 273.21 | 353.4 | < 1% | E |
| PERFLUORO-n-HEXANE | 355-42-0 | 100 | 4.8787E-09 | 2.9932E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-OCTANE | 307-34-6 | 100 | 6.8663E-11 | -3.6046E+04 | 0 | 5.5730E+06 | -2 | 298.15 | 298.15 | < 100% | E |
| 1,2-DIFLUORO-BENZENE | 367-11-3 | 101 | -6.6918E+00 | -5.9345E+02 | 0 | 0 | 0 | 298.15 | 322.89 | < 25% | E |
| FLUOROBENZENE | 462-06-6 | 101 | 2.9097E+00 | -6.4889E+03 | 0 | 9.4766E+05 | -2 | 273.15 | 353.15 | < 10% | E |
| HEXAFLUORO-BENZENE | 392-56-3 | 101 | 8.8895E+00 | -1.1813E+04 | 0 | 1.8684E+06 | -2 | 281.46 | 339.76 | < 3% | E |
| PERFLUORO-n-PENTANE | 678-26-2 | 100 | 7.2276E-08 | 3.2308E+03 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| PERFLUORO-n-HEPTANE | 335-57-9 | 100 | 5.6014E-10 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 100% | E |
| **C, H, I COMPOUNDS** | | | | | | | | | | | |
| METHYL IODIDE | 74-88-4 | 101 | 1.7790E+01 | -1.4071E+04 | 0 | 2.0544E+06 | -2 | 273.15 | 322.91 | < 5% | E |
| ETHYL IODIDE | 75-03-6 | 101 | 1.3260E+01 | -1.2282E+04 | 0 | 1.8002E+06 | -2 | 273.15 | 303.15 | < 3% | E |
| n-PROPYL IODIDE | 107-08-4 | 101 | -9.8622E+00 | 2.2204E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 5% | E |
| ISOPROPYL IODIDE | 75-30-9 | 101 | -1.0652E+01 | 5.4025E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| IODOBENZENE | 591-50-4 | 101 | 1.7033E+01 | -8.3179E+03 | 0 | 0 | 0 | 298 | 303.15 | < 10% | E |
| n-HEXYL IODIDE | 638-45-9 | 100 | 1.1954E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| n-BUTYL IODIDE | 542-69-8 | 100 | 2.2740E-05 | 1.2631E+04 | 3.2632E+01 | 0 | 0 | 298.15 | 298.15 | < 10% | S |
| **C, H, MULTIHALOGEN COMPOUNDS** | | | | | | | | | | | |
| DICHLORODIFLUORO-METHANE | 75-71-8 | 101 | -4.7872E+02 | 3.0993E+04 | 6.6398E+01 | -1.1878E+06 | -2 | 274 | 313.9 | < 3% | E |
| TRICHLOROFLUORO-METHANE | 75-69-4 | | | | | | | | | | |
| 1,1,2-TRICHLORO-TRIFLUOROETHANE | 76-13-1 | 101 | -1.2463E+01 | 5.4155E+02 | 0 | 0 | 0 | 275.15 | 303.15 | < 25% | E |
| **C, H, NO2 COMPOUNDS** | | | | | | | | | | | |
| NITROMETHANE | 75-52-5 | 101 | 1.5480E+01 | -1.0523E+04 | 0 | 1.4556E+06 | -2 | 273.15 | 363.15 | < 10% | E |
| NITROETHANE | 79-24-3 | 101 | 5.9340E+00 | -5.9512E+03 | 0 | 8.4315E+05 | -2 | 273.15 | 363.25 | < 5% | E |
| 1-NITROPROPANE | 108-03-2 | 101 | 6.2988E+00 | -7.1087E+03 | 0 | 1.0499E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| 2-NITROPROPANE | 79-46-9 | 101 | 4.1019E+00 | -5.7427E+03 | 0 | 8.4502E+05 | -2 | 292.85 | 363.35 | < 5% | E |
| 1-NITROBUTANE | 627-05-4 | 100 | 6.5301E-04 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| o-NITROTOLUENE | 88-72-2 | 101 | -5.7342E+00 | -1.0869E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| p-NITROTOLUENE | 99-99-0 | 101 | -2.6968E+00 | -2.1673E+03 | 0 | 0 | 0 | 281 | 338 | < 10% | E |
| m-NITROTOLUENE | 99-08-1 | 101 | -7.4215E+00 | -6.5552E+02 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| NITROBENZENE | 98-95-3 | 101 | 6.8466E+00 | -8.1755E+03 | 0 | 1.1026E+06 | -2 | 283.15 | 372.85 | < 5% | E |
| m-DINITROBENZENE | 99-65-0 | 101 | 1.3019E+00 | -3.2988E+03 | 0 | 0 | 0 | 277.65 | 310.15 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| p-DINITROBENZENE | 100-25-4 | 101 | -2.1454E+00 | -2.9164E+03 | 0 | 0 | 0 | 277.65 | 310.15 | < 5% | E |
| 2,4-DINITROTOLUENE | 121-14-2 | 101 | 2.8417E+01 | -1.9872E+04 | 0 | 2.4358E+06 | -2 | 277.15 | 334.95 | < 5% | E |
| 2,6-DINITROTOLUENE | 606-20-2 | 101 | 3.3784E+00 | -4.2272E+03 | 0 | 0 | 0 | 278 | 314 | < 5% | E |
| 3,4-DINITROTOLUENE | 610-39-9 | 101 | 2.0447E+00 | -3.8841E+03 | 0 | 0 | 0 | 278.2 | 313.2 | < 5% | E |
| 2,4,6-TRINITROTOLUENE | 118-96-7 | 101 | 3.5464E+01 | -2.4251E+04 | 0 | 3.0504E+06 | -2 | 275.55 | 334.15 | < 10% | E |
| RDX | 121-82-4 | 101 | 5.2818E+00 | -5.7566E+03 | 0 | 1.4123E+05 | -2 | 275.25 | 307.35 | < 5% | E |
| HMX | 2691-41-0 | 101 | 7.0734E+00 | -6.6105E+03 | 0 | 0 | 0 | 275.25 | 305.45 | < 10% | E |
| **C1/C2 ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| CARBON TETRACHLORIDE | 56-23-5 | 101 | 1.5476E+01 | -1.4953E+04 | 0 | 2.2550E+06 | -2 | 273.15 | 366.15 | < 5% | E |
| METHYL CHLORIDE | 74-87-3 | 101 | -2.8687E+00 | -4.8446E+03 | 0 | 1.1429E+06 | -2 | 273.15 | 366.15 | < 10% | E |
| ETHYL CHLORIDE | 75-00-3 | 101 | -1.8893E+02 | 1.0561E+04 | 2.5805E+01 | 0 | 0 | 285.45 | 366.15 | < 25% | E |
| VINYL CHLORIDE | 75-01-4 | 101 | -1.5752E+01 | 2.1198E+03 | 0 | 1.3139E+05 | -2 | 273.35 | 366.15 | < 25% | E |
| DICHLORO-METHANE | 75-09-2 | 101 | 1.4073E+00 | -3.8511E+03 | 0 | 5.3262E+05 | -2 | 273.15 | 366.15 | < 10% | E |
| CHLOROFORM | 67-66-3 | 101 | 6.1301E+00 | -7.9847E+03 | 0 | 1.2365E+06 | -2 | 273.15 | 366.15 | < 3% | E |
| 1,1-DICHLOROETHANE | 75-34-3 | 101 | 9.8021E+00 | -1.0195E+04 | 0 | 1.5486E+06 | -2 | 273.15 | 366.15 | < 5% | E |
| 1,2-DICHLOROETHANE | 107-06-2 | 101 | 1.1248E+01 | -1.0523E+04 | 0 | 1.5653E+06 | -2 | 273.15 | 366.15 | < 10% | E |
| 1,1,2-TRICHLOROETHANE | 79-00-5 | 101 | -1.4213E+00 | -3.2057E+03 | 0 | 4.2655E+05 | -2 | 273.15 | 363.95 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| HEXA-CHLOROETHANE | 67-72-1 | 101 | -1.0570E+01 | -6.4713E+02 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| 1,1,1-TRICHLORO-ETHANE | 71-55-6 | 101 | -7.0243E+00 | -1.1282E+03 | 0 | 1.9183E+05 | -2 | 273.15 | 348.15 | < 10% | E |
| 1,1,1,2-TETRACHLORO-ETHANE | 630-20-6 | 101 | 1.5281E+01 | -1.4390E+04 | 0 | 2.1225E+06 | -2 | 273.15 | 323.15 | < 10% | E |
| 1,1,2,2-TETRACHLORO-ETHANE | 79-34-5 | 101 | -7.3648E+00 | -2.1019E+02 | 0 | 0 | 0 | 283.15 | 328.65 | < 10% | E |
| TRICHLORO-ETHYLENE | 79-01-6 | 101 | 9.3855E+00 | -1.0828E+04 | 0 | 1.6277E+06 | -2 | 274.22 | 366.15 | < 5% | E |
| TETRACHLORO-ETHYLENE | 127-18-4 | 101 | 1.0289E+01 | -1.2404E+04 | 0 | 1.8415E+06 | -2 | 273.15 | 364.95 | < 10% | E |
| cis-1,2-DICHLORO-ETHYLENE | 156-59-2 | 101 | 6.5856E+00 | -8.1835E+03 | 0 | 1.2548E+06 | -2 | 281.15 | 366.15 | < 10% | E |
| trans-1,2-DICHLORO-ETHYLENE | 156-60-5 | 101 | -8.4863E+00 | 4.1422E+02 | 0 | 0 | 0 | 283.15 | 323.15 | < 10% | E |
| PENTACHLORO-ETHANE | 76-01-7 | 101 | -1.7027E+01 | 2.0331E+03 | 0 | 0 | 0 | 293.15 | 298 | < 25% | E |
| 1,1-DICHLORO-ETHYLENE | 75-35-4 | 101 | 1.0285E+01 | -1.1316E+04 | 0 | 1.7781E+06 | -2 | 275.15 | 363.65 | < 10% | E |
| **C3 & HIGHER ALIPHATIC CHLORIDES** | | | | | | | | | | | |
| 1,4-DICHLOROBUTANE | 110-56-5 | 101 | -2.1428E+00 | -1.9291E+03 | 0 | 0 | 0 | 286.65 | 298.05 | < 25% | E |
| 1,5-DICHLOROPENTANE | 628-76-2 | 101 | -3.5394E+00 | -2.1037E+03 | 0 | 0 | 0 | 274.15 | 295.85 | < 50% | E |
| 1,2-DICHLOROPROPANE | 78-87-5 | 101 | 9.0358E+00 | -9.7318E+03 | 0 | 1.4095E+06 | -2 | 273.15 | 353.35 | < 10% | E |
| ISOPROPYL CHLORIDE | 75-29-6 | 101 | -1.0554E+01 | 9.8685E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 10% | E |
| 1,2,3-TRICHLOROPROPANE | 96-18-4 | 101 | 3.9845E+00 | -3.6177E+03 | 0 | 0 | 0 | 275.05 | 318.15 | < 25% | E |
| HEXACHLORO-1,3-BUTADIENE | 87-68-3 | 101 | -1.0024E+01 | -1.4778E+03 | 0 | 0 | 0 | 275.15 | 298.15 | < 50% | E |

## Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PROPYL CHLORIDE | 540-54-5 | 101 | -1.0407E+01 | 9.0589E+02 | 0 | 0 | 0 | 273.15 | 310.15 | < 10% | E |
| n-BUTYL CHLORIDE | 109-69-3 | 101 | -1.0007E+01 | 3.3093E+02 | 0 | 0 | 0 | 273.35 | 310.15 | < 10% | E |
| sec-BUTYL CHLORIDE | 78-86-4 | 101 | -1.1014E+01 | 6.6934E+02 | 0 | 0 | 0 | 275.05 | 298.05 | < 10% | E |
| 1-CHLOROPENTANE | 543-59-9 | 101 | 1.6436E+01 | -1.5354E+04 | 0 | 2.2009E+06 | -2 | 275.65 | 310.15 | < 5% | E |
| 1,3-DICHLOROPROPANE | 142-28-9 | 101 | -2.5185E+00 | -1.6021E+03 | 0 | 0 | 0 | 275.05 | 303.15 | < 25% | E |
| **CYCLOALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| CYCLOHEXANOL | 108-93-0 | 6000 | -3.0993E+01 | 4.8212E+03 | 3.9172E-02 | -2.5974E+00 | 457.87 | 273.15 | 457.87 | < 10% | E |
| **CYCLOALKANES** | | | | | | | | | | | |
| CYCLOPENTANE | 287-92-3 | 101 | 8.0479E+00 | -1.0977E+04 | 0 | 1.6644E+06 | -2 | 298 | 426.25 | < 10% | E |
| CYCLOHEXANE | 110-82-7 | 101 | 1.1090E+01 | -1.3338E+04 | 0 | 1.9909E+06 | -2 | 274.25 | 424.15 | < 25% | E |
| CYCLOHEPTANE | 291-64-5 | 100 | 3.5216E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| CYCLOOCTANE | 292-64-8 | 101 | -3.5056E+00 | -5.6325E+03 | 0 | 7.6092E+05 | -2 | 274.15 | 313.15 | < 10% | E |
| **CYCLOALKENES** | | | | | | | | | | | |
| CYCLOPENTENE | 142-29-0 | 101 | -8.1547E+00 | -1.4308E+02 | 0 | 0 | 0 | 283.15 | 298.15 | < 50% | E |
| CYCLOHEXENE | 110-83-8 | 101 | -8.0999E+00 | -4.7103E+02 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| CYCLOHEPTENE | 628-92-2 | 100 | 1.2363E-05 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| CYCLOOCTENE | 931-88-4 | 101 | -1.0325E+01 | -6.4046E+02 | 0 | 0 | 0 | 274.15 | 313.15 | < 5% | E |
| | | | | | | | | | | | |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **DIALKENES** | | | | | | | | | | | |
| 1,4-CYCLOHEXADIENE | 628-41-1 | 101 | -7.5088E+00 | -2.9759E+02 | 0 | 0 | 0 | 278.26 | 318.36 | < 25% | E |
| **DICARBOXYLIC ACIDS** | | | | | | | | | | | |
| ADIPIC ACID | 124-04-9 | 101 | 3.5900E+01 | -2.0360E+04 | 0 | 2.3624E+06 | -2 | 278.15 | 338.15 | < 3% | E |
| SUCCINIC ACID | 110-15-6 | 101 | 1.1306E+01 | -5.6087E+03 | 0 | 2.8154E+05 | -2 | 278.15 | 338.15 | < 3% | E |
| GLUTARIC ACID | 110-94-1 | 101 | -2.4823E+03 | 2.1516E+05 | 3.4284E+02 | -1.7292E+07 | -2 | 276.55 | 342.15 | < 3% | E |
| **DIMETHYLALKANES** | | | | | | | | | | | |
| 2,2-DIMETHYLBUTANE | 75-83-2 | 100 | 4.4181E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | S |
| 2,3-DIMETHYLBUTANE | 79-29-8 | 101 | 1.6456E+01 | -1.7985E+04 | 0 | 2.7997E+06 | -2 | 273.15 | 422.65 | < 25% | E |
| 2,4-DIMETHYL-PENTANE | 108-08-7 | 100 | 7.3837E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| 3,3-DIMETHYL-PENTANE | 562-49-2 | 101 | -1.7960E+03 | 1.5381E+05 | 2.4627E+02 | -1.2163E+07 | -2 | 298.15 | 423.64 | < 25% | E |
| 2,2-DIMETHYLHEXANE | 590-73-8 | 101 | 2.9049E+01 | -2.6493E+04 | 0 | 3.9458E+06 | -2 | 274.35 | 313.15 | < 3% | E |
| 2,5-DIMETHYLHEXANE | 592-13-2 | 101 | 3.8363E+01 | -3.1483E+04 | 0 | 4.5955E+06 | -2 | 275.15 | 313.05 | < 3% | E |
| **DIPHENYL/POLYAROMATICS** | | | | | | | | | | | |
| BIPHENYL | 92-52-4 | 101 | 4.2986E+01 | -3.0707E+04 | 0 | 4.0885E+06 | -2 | 293.15 | 337.65 | < 10% | E |
| **EPOXIDES** | | | | | | | | | | | |
| 2-METHYL-TETRAHYDROFURAN | 96-47-9 | 101 | -1.0213E+01 | 2.0161E+03 | 0 | -4.0757E+03 | -2 | 273.15 | 343.75 | < 10% | E |
| TRIOXANE | 110-88-3 | 6000 | -5.1321E+02 | 7.6276E+04 | 8.5628E-01 | -2.5488E+00 | 321.65 | 293.15 | 321.65 | < 25% | E |
| TETRAHYDROPYRAN | 142-68-7 | 101 | -1.1151E+03 | 9.0997E+04 | 1.5415E+02 | -6.4427E+06 | -2 | 273.15 | 354.45 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DIBENZOFURAN | 132-64-9 | 101 | -1.3449E+00 | -3.9001E+03 | 0 | 0 | 0 | 278.15 | 318.15 | < 25% | E |
| **FORMATES** | | | | | | | | | | | |
| ETHYL FORMATE | 109-94-4 | 101 | 8.8137E+00 | -7.2082E+03 | 0 | 1.0206E+06 | -2 | 278.15 | 348.65 | < 3% | E |
| n-PROPYL FORMATE | 110-74-7 | 101 | 6.2828E+00 | -7.2734E+03 | 0 | 1.1493E+06 | -2 | 272.15 | 333.15 | < 10% | E |
| n-BUTYL FORMATE | 592-84-7 | 101 | -3.0776E+00 | -9.7124E+02 | 0 | 0 | 0 | 273.15 | 363.75 | < 25% | E |
| ISOBUTYL FORMATE | 542-55-2 | 101 | 1.6896E+00 | -5.6214E+03 | 0 | 9.5112E+05 | -2 | 273.15 | 333.55 | < 10% | E |
| n-PENTYL FORMATE | 638-49-3 | 101 | 6.3123E+00 | -9.0250E+03 | 0 | 1.4307E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| tert-BUTYL FORMATE | 762-75-4 | 101 | -3.8596E+00 | -5.9611E+02 | 0 | 0 | 0 | 278.15 | 308.15 | < 5% | E |
| **KETONES** | | | | | | | | | | | |
| METHYL ETHYL KETONE | 78-93-3 | 101 | -1.4231E+03 | 1.1758E+05 | 1.9698E+02 | -8.5370E+06 | -2 | 254.64 | 415.75 | < 5% | E |
| 3-PENTANONE | 96-22-0 | 101 | 6.6297E+00 | -7.9913E+03 | 0 | 1.3864E+06 | -2 | 273.15 | 353.35 | < 10% | E |
| METHYL ISOBUTYL KETONE | 108-10-1 | 101 | 2.6363E+00 | -6.2055E+03 | 0 | 1.1064E+06 | -2 | 273.15 | 363.55 | < 10% | E |
| 3-HEPTANONE | 106-35-4 | 101 | 4.8630E-01 | -5.8367E+03 | 0 | 1.0527E+06 | -2 | 273.15 | 363.25 | < 10% | E |
| 4-HEPTANONE | 123-19-3 | 101 | 4.6691E+00 | -8.4432E+03 | 0 | 1.4500E+06 | -2 | 273.15 | 363.35 | < 10% | E |
| 3-HEXANONE | 589-38-8 | 101 | -1.2639E+01 | 1.9983E+03 | 0 | 0 | 0 | 293.15 | 310.2 | < 25% | E |
| 2-PENTANONE | 107-87-9 | 101 | 3.8928E+00 | -6.2893E+03 | 0 | 1.1324E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| METHYL ISOPROPYL KETONE | 563-80-4 | 101 | -4.6269E+02 | 3.2695E+04 | 6.4733E+01 | -1.7848E+06 | -2 | 265.15 | 453.15 | < 10% | E |
| 2-HEXANONE | 591-78-6 | 101 | 2.9923E+00 | -6.5018E+03 | 0 | 1.1514E+06 | -2 | 273.15 | 364.65 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-HEPTANONE | 110-43-0 | 101 | 6.4375E+00 | -9.3023E+03 | 0 | 1.5481E+06 | -2 | 273.15 | 363.65 | < 5% | E |
| 5-METHYL-2-HEXANONE | 110-12-3 | 101 | 7.1688E+00 | -9.6863E+03 | 0 | 1.6139E+06 | -2 | 273.15 | 362.85 | < 5% | E |
| 3,3-DIMETHYL-2-BUTANONE | 75-97-8 | 101 | -8.1543E-01 | -4.0863E+03 | 0 | 7.8661E+05 | -2 | 273.15 | 363.35 | < 5% | E |
| DIISOBUTYL KETONE | 108-83-8 | 101 | 7.1063E+00 | -1.1438E+04 | 0 | 1.9006E+06 | -2 | 273.15 | 363.85 | < 10% | E |
| DIISOPROPYL KETONE | 565-80-0 | 101 | -2.1253E+00 | -4.1921E+03 | 0 | 8.0333E+05 | -2 | 273.15 | 363.45 | < 10% | E |
| 5-NONANONE | 502-56-7 | 101 | 1.7303E+00 | -8.2199E+03 | 0 | 1.4280E+06 | -2 | 273.15 | 363.75 | < 25% | E |
| 2-NONANONE | 821-55-6 | 101 | 5.8740E+00 | -1.0490E+04 | 0 | 1.7112E+06 | -2 | 273.15 | 364.35 | < 25% | E |
| ACETYLACETONE | 123-54-6 | 101 | 1.6717E+01 | -1.1122E+04 | 0 | 1.5290E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| ISOPHORONE | 78-59-1 | 101 | 9.5687E+00 | -1.0617E+04 | 0 | 1.7565E+06 | -2 | 273.15 | 364.25 | < 5% | E |
| CYCLOPENTANONE | 120-92-3 | 6000 | -1.6081E+01 | 3.1202E+03 | 1.6210E-02 | -2.9219E+00 | 378.15 | 267.45 | 378.15 | < 3% | E |
| CYCLOHEXANONE | 108-94-1 | 101 | 6.6031E+00 | -7.5035E+03 | 0 | 1.2904E+06 | -2 | 273.15 | 363.85 | < 5% | E |
| 2-OCTANONE | 111-13-7 | 101 | 7.7020E+00 | -1.1250E+04 | 0 | 1.9033E+06 | -2 | 273.15 | 364.15 | < 25% | E |
| ACETOPHENONE | 98-86-2 | 101 | 2.1398E+00 | -4.5194E+03 | 0 | 5.3558E+05 | -2 | 293.05 | 353.35 | < 25% | E |
| 3-OCTANONE | 106-68-3 | 101 | -1.6485E+00 | -5.0117E+03 | 0 | 8.7634E+05 | -2 | 273.15 | 364.15 | < 10% | E |
| 3-NONANONE | 925-78-0 | 101 | -9.4462E+00 | -6.6198E+01 | 0 | 0 | 0 | 273.15 | 353.35 | < 25% | E |
| 2,6,8-TRIMETHYL-4-NONANONE | 123-18-2 | 100 | 2.2065E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 25% | P |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **MERCAPTANS** | | | | | | | | | | | |
| ISOPROPYL MERCAPTAN | 75-33-2 | 101 | -7.3515E+00 | 9.3654E+01 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| n-BUTYL MERCAPTAN | 109-79-5 | 101 | 1.8888E+01 | -1.6328E+04 | 0 | 2.4137E+06 | -2 | 288.15 | 333.15 | < 5% | E |
| **METHYLALKANES** | | | | | | | | | | | |
| 2-METHYLPENTANE | 107-83-5 | 101 | 1.6772E+01 | -1.8364E+04 | 0 | 2.8566E+06 | -2 | 273.15 | 422.65 | < 25% | E |
| 3-METHYLPENTANE | 96-14-0 | 100 | 2.7067E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 3% | S |
| 2-METHYLHEXANE | 591-76-4 | 100 | 4.5667E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| 3-METHYLHEXANE | 589-34-4 | 100 | 4.7716E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| 3-METHYLHEPTANE | 589-81-1 | 100 | 1.2491E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| 4-METHYLHEPTANE | 589-53-7 | 100 | 1.3224E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 5% | E |
| **N-ALCOHOLS** | | | | | | | | | | | |
| 1-BUTANOL | 71-36-3 | 6000 | -1.6135E+01 | 3.2105E+03 | 1.5570E-02 | -5.1405E+00 | 398.31 | 273.15 | 398.3 | < 3% | E |
| 1-PENTANOL | 71-41-0 | 101 | 7.8962E+00 | -8.7669E+03 | 0 | 1.4281E+06 | -2 | 273.15 | 368.95 | < 3% | E |
| 1-HEXANOL | 111-27-3 | 101 | 8.2658E+00 | -9.8737E+03 | 0 | 1.5999E+06 | -2 | 273.15 | 363.45 | < 10% | E |
| 1-HEPTANOL | 111-70-6 | 101 | 1.8876E+01 | -1.7053E+04 | 0 | 2.6686E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| 1-OCTANOL | 111-87-5 | 101 | 1.8301E+01 | -1.7025E+04 | 0 | 2.5985E+06 | -2 | 288.15 | 363.45 | < 10% | EP |
| 1-NONANOL | 143-08-8 | 101 | 1.8177E+01 | -1.7366E+04 | 0 | 2.5783E+06 | -2 | 288.15 | 363.15 | < 25% | E |
| 1-DECANOL | 112-30-1 | 101 | 2.2457E+01 | -2.0308E+04 | 0 | 2.9573E+06 | -2 | 288.15 | 363.15 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-UNDECANOL | 112-42-5 | 100 | 1.0330E-06 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-DODECANOL | 112-53-8 | 100 | 2.5520E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-TRIDECANOL | 112-70-9 | 100 | 6.3040E-08 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-TETRADECANOL | 112-72-1 | 100 | 1.5573E-08 | -2.1975E+04 | -4.5599E+01 | 0 | 0 | 298.15 | 298.15 | < 50% | P |
| 1-PENTADECANOL | 629-76-5 | 100 | 3.8469E-09 | -1.1094E+04 | -3.2981E+01 | 0 | 0 | 298.15 | 298.15 | < 100% | P |
| 1-HEXADECANOL | 36653-82-4 | 100 | 9.5034E-10 | -7.2665E+03 | 0 | 1.0944E+06 | -2 | 298.15 | 298.15 | < 100% | P |
| 1-HEPTADECANOL | 1454-85-9 | 100 | 2.3477E-10 | -1.2866E+04 | -2.5451E+01 | 0 | 0 | 298.15 | 298.15 | < 100% | P |
| 1-OCTADECANOL | 112-92-5 | 100 | 5.7993E-11 | -5.9638E+03 | -1.8057E+01 | 0 | 0 | 298.15 | 298.15 | < 100% | P |
| **N-ALIPHATIC PRIMARY AMINES** | | | | | | | | | | | |
| METHYLAMINE | 74-89-5 | 100 | 1 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | U | E |
| ETHYLAMINE | 75-04-7 | 100 | 1 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | U | E |
| n-PROPYLAMINE | 107-10-8 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 321.15 | U | E |
| n-BUTYLAMINE | 109-73-9 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 351.15 | U | E |
| n-PENTYLAMINE | 110-58-7 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 368.15 | U | E |
| **N-ALKANES** | | | | | | | | | | | |
| n-PENTANE | 109-66-0 | 101 | -1.3911E+03 | 1.1170E+05 | 1.9221E+02 | -8.0108E+06 | -2 | 273.15 | 422.65 | < 25% | E |
| n-HEXANE | 110-54-3 | 101 | -5.9005E+02 | 3.7354E+04 | 8.2875E+01 | -1.8163E+06 | -2 | 273.15 | 443.15 | < 10% | E |
| n-HEPTANE | 142-82-5 | 101 | -6.1790E+02 | 3.9030E+04 | 8.6780E+01 | -1.9566E+06 | -2 | 273.15 | 443.75 | < 25% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-OCTANE | 111-65-9 | 101 | 2.6143E+01 | -2.5670E+04 | 0 | 3.9079E+06 | -2 | 273.15 | 456.15 | < 25% | E |
| n-NONANE | 111-84-2 | 101 | 4.0403E+01 | -3.6046E+04 | 0 | 5.5730E+06 | -2 | 287.95 | 409.75 | < 50% | E |
| n-DECANE | 124-18-5 | 100 | 4.3460E-09 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 50% | S |
| **N-ALKYLBENZENES** | | | | | | | | | | | |
| BENZENE | 71-43-2 | 101 | 8.8569E+00 | -9.5142E+03 | 0 | 1.3553E+06 | -2 | 273.15 | 527.15 | < 3% | E |
| TOLUENE | 108-88-3 | 101 | 8.9793E+00 | -1.0140E+04 | 0 | 1.4189E+06 | -2 | 261.7 | 473.55 | < 5% | E |
| ETHYLBENZENE | 100-41-4 | 101 | 1.4054E+01 | -1.4454E+04 | 0 | 2.1340E+06 | -2 | 273.15 | 373.15 | < 5% | E |
| n-PROPYLBENZENE | 103-65-1 | 101 | 4.5679E+00 | -8.9194E+03 | 0 | 1.2076E+06 | -2 | 273.65 | 328.15 | < 10% | E |
| n-BUTYLBENZENE | 104-51-8 | 101 | 1.7850E+01 | -1.7506E+04 | 0 | 2.4576E+06 | -2 | 273.65 | 373.15 | < 5% | E |
| n-HEPTYLBENZENE | 1078-71-3 | 100 | 2.3098E-08 | -1.0897E+04 | -3.2652E+01 | 0 | 0 | 298.15 | 298.15 | < 5% | P |
| n-DECYLBENZENE | 104-72-3 | 100 | 2.0688E-10 | -9.7708E+03 | -4.2873E+01 | 3.6254E-02 | 1 | 298.15 | 298.15 | < 10% | S |
| n-PENTYLBENZENE | 538-68-1 | 101 | 1.1262E+01 | -1.4633E+04 | 0 | 2.0603E+06 | -2 | 280.15 | 318.15 | < 10% | E |
| n-HEXYLBENZENE | 1077-16-3 | 101 | 6.7333E+00 | -1.2793E+04 | 0 | 1.7900E+06 | -2 | 278.15 | 318.15 | < 3% | E |
| n-OCTYLBENZENE | 2189-60-8 | 100 | 4.9663E-09 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| n-NONYLBENZENE | 1081-77-2 | 100 | 1.0313E-09 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | P |
| **NAPHTHALENES** | | | | | | | | | | | |
| NAPHTHALENE | 91-20-3 | 101 | 2.0659E+01 | -1.6308E+04 | 0 | 1.9288E+06 | -2 | 275.05 | 346.55 | < 3% | E |
| 1-METHYL-NAPHTHALENE | 90-12-0 | 101 | -8.4391E+00 | -1.2142E+03 | 0 | 0 | 0 | 277.25 | 304.85 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2-METHYL-NAPHTHALENE | 91-57-6 | 101 | -2.6452E+00 | -3.0013E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| 1-ETHYL-NAPHTHALENE | 1127-76-0 | 101 | -7.4377E+00 | -1.8483E+03 | 0 | 0 | 0 | 281.55 | 304.85 | < 10% | E |
| **NITRILES** | | | | | | | | | | | |
| PROPIONITRILE | 107-12-0 | 101 | 1.5998E+01 | -1.1438E+04 | 0 | 1.6904E+06 | -2 | 298.15 | 353.15 | < 5% | E |
| ACRYLONITRILE | 107-13-1 | 101 | 5.6317E+00 | -5.4279E+03 | 0 | 7.8429E+05 | -2 | 273.15 | 343.15 | < 5% | E |
| METHACRYLO-NITRILE | 126-98-7 | 101 | 1.2848E+01 | -1.0849E+04 | 0 | 1.6366E+06 | -2 | 273.15 | 353.15 | < 10% | E |
| SUCCINONITRILE | 110-61-2 | 6000 | 1.4744E+02 | -2.4452E+04 | -2.2705E-01 | -3.3471E+00 | 329.01 | 305 | 329 | < 3% | E |
| GLUTARONITRILE | 544-13-8 | 5000 | -1.3892E+04 | 8.9362E+04 | 2.0360E+03 | 1.7487E+03 | 342.00 | 290 | 342 | < 10% | E |
| n-BUTYRONITRILE | 109-74-0 | 101 | 1.1169E+00 | -3.7470E+03 | 0 | 5.9779E+05 | -2 | 273.15 | 363.15 | < 3% | E |
| VALERONITRILE | 110-59-8 | 101 | 1.5015E+01 | -1.2632E+04 | 0 | 1.9077E+06 | -2 | 273.15 | 363.15 | < 10% | E |
| ISOBUTYRO-NITRILE | 78-82-0 | 101 | -4.5050E-01 | -2.6707E+03 | 0 | 4.2005E+05 | -2 | 273.15 | 363.15 | < 5% | E |
| BENZONITRILE | 100-47-0 | 101 | -3.8294E+00 | -1.0182E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 25% | E |
| VINYL-ACETONITRILE | 109-75-1 | 101 | 9.3859E+00 | -8.2424E+03 | 0 | 1.2031E+06 | -2 | 273.15 | 363.15 | < 5% | E |
| PHENYL-ACETONITRILE | 140-29-4 | 101 | 1.5843E+01 | -1.3292E+04 | 0 | 1.8234E+06 | -2 | 273.15 | 363.15 | < 25% | E |
| **NITROAMINES** | | | | | | | | | | | |
| o-NITROANILINE | 88-74-4 | 101 | 7.2633E+00 | -4.8220E+03 | 0 | 0 | 0 | 298.15 | 313.25 | < 50% | E |
| p-NITROANILINE | 100-01-6 | 101 | 7.2258E+00 | -4.9899E+03 | 0 | 0 | 0 | 293.15 | 313.25 | < 10% | E |
| m-NITROANILINE | 99-09-2 | 6000 | 2.2651E+00 | -3.5004E+03 | 5.9660E-03 | -1.8641E+00 | 458.36 | 273.15 | 458.35 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **ORGANIC SALTS** | | | | | | | | | | | |
| DIETHYL CARBONATE | 105-58-8 | 101 | 6.3888E+00 | -8.1262E+03 | 0 | 1.3289E+06 | -2 | 273.15 | 363.45 | < 5% | E |
| DIMETHYL CARBONATE | 616-38-6 | 101 | 4.6151E+00 | -4.7448E+03 | 0 | 6.8616E+05 | -2 | 282.95 | 333.55 | < 3% | E |
| **OTHER ALIPHATIC ALCOHOLS** | | | | | | | | | | | |
| 2-METHYL-1-PROPANOL | 78-83-1 | 101 | -2.3310E+03 | 1.9509E+05 | 3.2240E+02 | -1.4587E+07 | -2 | 273.15 | 407.25 | < 10% | E |
| 2-BUTANOL | 78-92-2 | 6000 | -2.3732E+01 | 4.4883E+03 | 2.6387E-02 | -3.5525E+00 | 386.65 | 273.15 | 386.65 | < 3% | E |
| 2-PENTANOL | 6032-29-7 | 101 | 6.9003E+00 | -8.2230E+03 | 0 | 1.4184E+06 | -2 | 273.15 | 363.45 | < 5% | E |
| 2-METHYL-2-BUTANOL | 75-85-4 | 101 | -1.8723E+03 | 1.5768E+05 | 2.5837E+02 | -1.1765E+07 | -2 | 273.65 | 401.75 | < 10% | E |
| 2-METHYL-1-BUTANOL | 137-32-6 | 101 | 8.0268E+00 | -8.9236E+03 | 0 | 1.4838E+06 | -2 | 273.65 | 363.95 | < 5% | E |
| 2,2-DIMETHYL-1-PROPANOL | 75-84-3 | 101 | 4.5624E+00 | -6.9514E+03 | 0 | 1.2234E+06 | -2 | 285.15 | 363.15 | < 10% | E |
| 2-HEXANOL | 626-93-7 | 101 | 7.9408E+00 | -9.6532E+03 | 0 | 1.6249E+06 | -2 | 273.15 | 363.35 | < 10% | E |
| 3-HEXANOL | 623-37-0 | 101 | 6.2630E+00 | -8.7820E+03 | 0 | 1.5363E+06 | -2 | 273.15 | 363.45 | < 5% | E |
| 3-METHYL-1-PENTANOL | 589-35-5 | 101 | 1.0298E+01 | -1.0896E+04 | 0 | 1.7641E+06 | -2 | 273.15 | 363.65 | < 5% | E |
| 3-METHYL-3-PENTANOL | 77-74-7 | 101 | -9.2854E+00 | 1.2486E+03 | 0 | 0 | 0 | 282.95 | 363.55 | < 10% | E |
| 3-PENTANOL | 584-02-1 | 101 | 7.0880E+00 | -8.4508E+03 | 0 | 1.4859E+06 | -2 | 273.15 | 363.15 | < 5% | E |
| 3-METHYL-1-BUTANOL | 123-51-3 | 101 | 5.1443E+00 | -7.1281E+03 | 0 | 1.2022E+06 | -2 | 273.15 | 363.15 | < 5% | E |
| 3-METHYL-2-BUTANOL | 598-75-4 | 101 | -1.3435E+03 | 1.1083E+05 | 1.8565E+02 | -8.0438E+06 | -2 | 273.15 | 363.15 | < 5% | E |
| 2-HEPTANOL | 543-49-7 | 101 | 8.9387E+00 | -1.1008E+04 | 0 | 1.8246E+06 | -2 | 273.15 | 363.35 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3-HEPTANOL | 589-82-2 | 101 | 5.5168E+00 | -9.1575E+03 | 0 | 1.5956E+06 | -2 | 273.15 | 363.35 | < 10% | E |
| 4-METHYL-2-PENTANOL | 108-11-2 | 101 | 5.0667E+00 | -7.8098E+03 | 0 | 1.3557E+06 | -2 | 273.15 | 363.35 | < 10% | E |
| 2-OCTANOL | 123-96-6 | 101 | 1.6068E+01 | -1.6328E+04 | 0 | 2.6604E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| 2-NONANOL | 628-99-9 | 101 | 1.3272E+01 | -1.5882E+04 | 0 | 2.6529E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| 2,6-DIMETHYL-4-HEPTANOL | 108-82-7 | 101 | -3.2973E+00 | -5.3209E+03 | 0 | 1.0358E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| **OTHER ALIPHATIC AMINES** | | | | | | | | | | | |
| TRIETHYLAMINE | 121-44-8 | 6000 | 2.7364E+01 | -5.2885E+03 | -3.9158E-02 | -7.5913E+00 | 291.14 | 291.15 | 353.15 | < 25% | E |
| DI-n-PROPYLAMINE | 142-84-7 | 6000 | 1.1999E+01 | -2.2185E+03 | -2.2788E-02 | -5.6220E+00 | 268.34 | 268.35 | 363.15 | < 25% | E |
| N,N-DIMETHYL-n-BUTYLAMINE | 927-62-8 | 6000 | -2.4897E+01 | 4.2843E+03 | 1.9112E-02 | -1.2491E+00 | 276.94 | 276.95 | 363.15 | < 25% | E |
| N,N-DIETHYL-METHYLAMINE | 616-39-7 | 6000 | 3.7296E+02 | -6.6421E+04 | -5.2238E-01 | -1.0773E+01 | 322.05 | 322.06 | 351.43 | < 25% | E |
| DIETHYLAMINE | 109-89-7 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 328.15 | U | E |
| DIISOPROPYLAMINE | 108-18-9 | 6000 | 1.2988E+02 | -2.2447E+04 | -1.9105E-01 | -8.2043E+00 | 300.17 | 300.18 | 357.15 | < 25% | E |
| DI-n-BUTYLAMINE | 111-92-2 | 101 | 4.2595E+00 | -9.3265E+03 | 0 | 1.7549E+06 | -2 | 273.15 | 363.15 | < 10% | E |
| TRI-n-BUTYLAMINE | 102-82-9 | 101 | -1.3391E+01 | 1.1860E+03 | 0 | 0 | 0 | 273.15 | 353.15 | < 25% | E |
| **OTHER ALKANES** | | | | | | | | | | | |
| 2,3,4-TRIMETHYL-PENTANE | 565-75-3 | 100 | 2.1260E-07 | 1.1974E+04 | 3.1657E+01 | 0 | 0 | 298.15 | 298.15 | < 5% | S |
| 2,2,5-TRIMETHYL-HEXANE | 3522-94-9 | 101 | -2.0551E+01 | 1.2394E+03 | 0 | 0 | 0 | 273.15 | 298.15 | < 5% | E |
| | | | | | | | | | | | |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **OTHER ALKYLBENZENES** | | | | | | | | | | | |
| o-XYLENE | 95-47-6 | 101 | 1.2005E+01 | -1.2703E+04 | 0 | 1.8021E+06 | -2 | 273.15 | 353.15 | < 10% | E |
| m-XYLENE | 108-38-3 | 101 | 1.1687E+01 | -1.2479E+04 | 0 | 1.7520E+06 | -2 | 273.15 | 543.75 | < 10% | E |
| p-XYLENE | 106-42-3 | 101 | 1.2851E+01 | -1.3397E+04 | 0 | 1.9251E+06 | -2 | 273.15 | 568.05 | < 10% | E |
| CUMENE | 98-82-8 | 101 | -9.0761E+00 | -7.3125E+02 | 0 | 0 | 0 | 288.15 | 318.15 | < 10% | E |
| 1,2,3-TRIMETHYL-BENZENE | 526-73-8 | 101 | -7.7694E+00 | -1.1242E+03 | 0 | 0 | 0 | 288.15 | 318.15 | < 25% | E |
| 1,2,4-TRIMETHYL-BENZENE | 95-63-6 | 101 | -8.3822E+00 | -9.8904E+02 | 0 | 0 | 0 | 288.15 | 318.15 | < 5% | E |
| MESITYLENE | 108-67-8 | 101 | 6.7148E+00 | -9.8463E+03 | 0 | 1.2888E+06 | -2 | 283.15 | 373.15 | < 25% | E |
| p-DIETHYLBENZENE | 105-05-5 | 100 | 3.3752E-06 | -2.0510E+04 | -3.8180E+01 | 0 | 0 | 293.15 | 293.15 | < 100% | E |
| 1,2,3,4-TETRAMETHYL-BENZENE | 488-23-3 | 101 | -1.0237E+01 | -8.1465E+02 | 0 | 0 | 0 | 288.15 | 308.15 | < 100% | E |
| 1,2,4,5-TETRAMETHYL-BENZENE | 95-93-2 | 100 | 4.6710E-07 | 0 | 0 | 0 | 0 | 298.15 | 298.15 | < 10% | E |
| **OTHER AMINES, IMINES** | | | | | | | | | | | |
| CYCLOHEXYL-AMINE | 108-91-8 | 100 | 1 | 0 | 0 | 0 | 0 | 273.15 | 363.15 | U | E |
| HEXAMETHYLENE-TETRAMINE | 100-97-0 | 101 | -2.8632E+00 | 1.4809E+02 | 0 | 0 | 0 | 293.15 | 353.15 | < 3% | E |
| N-ETHYL-2-METHYLALLYL-AMINE | 18328-90-0 | 6000 | -5.2494E+01 | 9.2838E+03 | 5.8177E-02 | -4.3737E-02 | 291.76 | 291.75 | 363.15 | < 25% | E |
| TRIALLYLAMINE | 102-70-5 | 101 | 1.2461E+01 | -1.3869E+04 | 0 | 2.3202E+06 | -2 | 273.15 | 363.15 | < 25% | E |
| N-METHYL-CYCLOHEXYLAMINE | 100-60-7 | 6000 | -2.1877E+01 | 2.8736E+03 | 2.7524E-02 | -2.7938E+00 | 284.74 | 284.75 | 363.15 | < 3% | E |
| DIALLYLAMINE | 124-02-7 | 101 | 1.2788E+01 | -1.3282E+04 | 0 | 2.4774E+06 | -2 | 279.15 | 363.15 | < 25% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| N-METHYLPIPERIDINE | 626-67-5 | 6000 | -2.6040E+01 | 3.9739E+03 | 3.2166E-02 | -3.2579E+00 | 317.14 | 317.15 | 363.15 | < 10% | E |
| **OTHER CONDENSED RINGS** | | | | | | | | | | | |
| FLUORANTHENE | 206-44-0 | 101 | 3.6246E-01 | -5.3775E+03 | 0 | 0 | 0 | 281.25 | 333.15 | < 10% | E |
| FLUORENE | 86-73-7 | 101 | -4.1946E-01 | -4.4885E+03 | 0 | 0 | 0 | 279.75 | 333.15 | < 10% | E |
| ANTHRACENE | 120-12-7 | 101 | 2.3500E+01 | -1.9563E+04 | 0 | 2.0384E+06 | -2 | 273.45 | 347.85 | < 5% | E |
| PHENANTHRENE | 85-01-8 | 101 | 1.9291E+01 | -1.6237E+04 | 0 | 1.6996E+06 | -2 | 277.15 | 346.55 | < 5% | E |
| CHRYSENE | 218-01-9 | 101 | -8.7436E+00 | -4.1710E+03 | 0 | 0 | 0 | 279.65 | 302.15 | < 25% | E |
| PYRENE | 129-00-0 | 101 | 2.0676E+01 | -1.8288E+04 | 0 | 1.9905E+06 | -2 | 277.85 | 347.85 | < 5% | E |
| ACENAPHTHENE | 83-32-9 | 101 | 2.2202E+00 | -5.0460E+03 | 0 | 0 | 0 | 277.25 | 347.85 | < 25% | E |
| ACENAPHTHALENE | 208-96-8 | 101 | -4.9130E+00 | -2.5248E+03 | 0 | 0 | 0 | 277.25 | 304.15 | < 25% | E |
| BENZO[a]PYRENE | 50-32-8 | 101 | -6.0895E+00 | -5.0166E+03 | 0 | 0 | 0 | 281.15 | 308.15 | < 10% | E |
| BENZANTHRACENE | 56-55-3 | 101 | 1.1722E+02 | -7.6026E+04 | 0 | 1.0373E+07 | -2 | 276.85 | 308.15 | < 10% | E |
| BENZO[b]FLUORANTHENE | 205-99-2 | 101 | 6.9573E+00 | -8.9149E+03 | 0 | 0 | 0 | 283.15 | 328.15 | < 10% | E |
| **OTHER ETHERS/DIETHERS** | | | | | | | | | | | |
| METHYLAL | 109-87-5 | 101 | -3.7046E+00 | 3.8855E+02 | 0 | 0 | 0 | 273.15 | 313.15 | < 10% | E |
| 1,2-DIMETHOXYETHANE | 110-71-4 | 101 | -5.6795E+00 | 8.8936E+02 | 0 | 0 | 0 | 273.15 | 313.15 | < 25% | E |
| DIETHYLENE GLYCOL DIETHYL ETHER | 112-36-7 | 6000 | -6.1762E+01 | 1.1670E+04 | 6.9790E-02 | 4.4908E-02 | 301.14 | 301.15 | 363.25 | < 10% | E |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 112-73-2 | 101 | 1.4893E+01 | -1.7993E+04 | 0 | 3.2683E+06 | -2 | 273.15 | 363.15 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ANISOLE | 100-66-3 | 101 | -3.7251E+00 | -1.3661E+03 | 0 | 0 | 0 | 275.15 | 363.85 | < 5% | E |
| DIPHENYL ETHER | 101-84-8 | 100 | 1.9486E-06 | -1.1616E+04 | -2.9743E+01 | 0 | 0 | 298.15 | 298.15 | < 5% | S |
| 1,2-DIETHOXYETHANE | 629-14-1 | 101 | -1.6857E+01 | 5.9191E+03 | 0 | -5.6886E+05 | -2 | 273.15 | 363.15 | < 5% | E |
| **OTHER MONOAROMATICS** | | | | | | | | | | | |
| STYRENE | 100-42-5 | 101 | -4.2008E+00 | -1.6858E+03 | 0 | 0 | 0 | 293.32 | 313.02 | < 5% | E |
| **OTHER POLYFUNCTIONAL C, H, O** | | | | | | | | | | | |
| FURFURAL | 98-01-1 | 6000 | -1.8103E+01 | 2.6482E+03 | 2.4606E-02 | -3.5623E+00 | 394.05 | 273.15 | 394.05 | < 5% | E |
| 2-BUTOXYETHANOL | 111-76-2 | 101 | 6.8405E+01 | -5.1749E+04 | 0 | 9.2209E+06 | -2 | 322.15 | 401.15 | < 10% | E |
| 2-HEXOXYETHANOL | 112-25-4 | 101 | 1.1508E+01 | -1.3242E+04 | 0 | 2.3543E+06 | -2 | 273.15 | 363.15 | < 25% | E |
| 2-(2-HEXOXYETHOXY)-ETHANOL | 112-59-4 | 101 | 4.5719E+01 | -3.4663E+04 | 0 | 5.7078E+06 | -2 | 285.15 | 363.15 | < 25% | E |
| VANILLIN | 121-33-5 | 101 | -2.5626E+01 | 1.5128E+04 | 0 | -2.8283E+06 | -2 | 293.15 | 318.15 | < 3% | E |
| PROPYLENE GLYCOL n-BUTYL ETHER | 5131-66-8 | 101 | -1.8709E+00 | -3.8554E+03 | 0 | 8.8426E+05 | -2 | 268.15 | 363.15 | < 10% | E |
| **OTHER POLYFUNCTIONAL ORGANICS** | | | | | | | | | | | |
| MALATHION | 121-75-5 | 101 | -9.4825E+00 | -6.5710E+02 | 0 | 0 | 0 | 283.15 | 303.15 | < 25% | E |
| THIOUREA | 62-56-6 | 101 | -1.2285E+00 | 2.9718E+03 | 0 | -1.0679E+06 | -2 | 290.75 | 358.15 | < 1% | E |
| **OTHER SATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ISOVALERATE | 108-64-5 | 101 | 3.2211E+00 | -7.9778E+03 | 0 | 1.3642E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| DIETHYL MALONATE | 105-53-3 | 101 | 9.1270E+00 | -9.7095E+03 | 0 | 1.5509E+06 | -2 | 273.15 | 363.75 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DIETHYL SUCCINATE | 123-25-1 | 101 | 6.8326E+00 | -8.6091E+03 | 0 | 1.4125E+06 | -2 | 273.15 | 363.85 | < 10% | E |
| ETHYL TRIMETHYL ACETATE | 3938-95-2 | 101 | 1.5042E-01 | -6.4989E+03 | 0 | 1.1890E+06 | -2 | 273.15 | 363.55 | < 25% | E |
| DIMETHYL SUCCINATE | 106-65-0 | 101 | 7.0324E+00 | -6.6630E+03 | 0 | 1.0004E+06 | -2 | 293.75 | 364.75 | < 3% | E |
| DIMETHYL-MALONATE | 108-59-8 | 101 | 1.2864E+01 | -9.3645E+03 | 0 | 1.3133E+06 | -2 | 273.15 | 363.35 | < 10% | E |
| **POLYFUNCTIONAL ACIDS** | | | | | | | | | | | |
| SALICYLIC ACID | 69-72-7 | 101 | 2.8389E+01 | -1.8578E+04 | 0 | 2.2896E+06 | -2 | 273.08 | 348.15 | < 5% | E |
| **POLYFUNCTIONAL AMIDES/AMINES** | | | | | | | | | | | |
| UREA | 57-13-6 | 101 | 3.6465E+00 | -1.5491E+03 | 0 | 1.7577E+04 | -2 | 273.15 | 373.15 | < 3% | E |
| ACETAMIDE | 60-35-5 | 101 | 5.4067E+00 | -2.3153E+03 | 0 | 1.3645E+05 | -2 | 273.15 | 336.15 | < 3% | E |
| N,N-DIETHYL-HYDROXYLAMINE | 3710-84-7 | 101 | -6.6884E+02 | 5.7896E+04 | 9.1700E+01 | -4.4550E+06 | -2 | 273.15 | 363.15 | < 3% | E |
| **POLYFUNCTIONAL C, H, N, HALIDE, (O)** | | | | | | | | | | | |
| o-CHLOROANILINE | 95-51-2 | 101 | 1.3102E+01 | -1.2484E+04 | 0 | 1.9616E+06 | -2 | 298.15 | 431.15 | < 10% | E |
| p-CHLORONITRO-BENZENE | 100-00-5 | 101 | -1.8812E+00 | -2.5635E+03 | 0 | 0 | 0 | 283.15 | 313.15 | < 10% | E |
| **POLYFUNCTIONAL C, H, O, HALIDE** | | | | | | | | | | | |
| DI(2-CHLOROETHYL)-ETHER | 111-44-4 | 101 | 5.3292E+00 | -7.1469E+03 | 0 | 1.0658E+06 | -2 | 273.15 | 364.85 | < 5% | E |
| ETHYL-CHLOROACETATE | 105-39-5 | 101 | 6.9181E+00 | -8.0820E+03 | 0 | 1.2777E+06 | -2 | 273.15 | 363.65 | < 10% | E |
| o-CHLOROPHENOL | 95-57-8 | 6000 | -1.1011E+01 | 1.0640E+03 | 1.3317E-02 | -3.2801E+00 | 446.15 | 288.55 | 446.15 | < 5% | E |
| m-CHLOROPHENOL | 108-43-0 | 6000 | -5.3005E+00 | 2.3222E+02 | 5.1282E-03 | -4.2920E+00 | 403.96 | 298.15 | 403.95 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| p-CHLOROPHENOL | 106-48-9 | 6000 | -1.6519E+01 | 2.3389E+03 | 2.0971E-02 | -5.1532E+00 | 402.41 | 272.95 | 402.4 | < 25% | E |
| METHYL CHLOROACETATE | 96-34-4 | 101 | 5.2524E+00 | -5.9225E+03 | 0 | 8.7840E+05 | -2 | 273.15 | 363.25 | < 5% | E |
| **POLYFUNCTIONAL C, H, O, N** | | | | | | | | | | | |
| ACETAMINOPHEN | 103-90-2 | 101 | 3.0067E+01 | -1.9166E+04 | 0 | 2.4749E+06 | -2 | 278.15 | 343.15 | < 5% | E |
| ACETANILIDE | 103-84-4 | 101 | 2.3705E+00 | -2.8256E+03 | 0 | 0 | 0 | 293.15 | 303.15 | < 25% | E |
| **POLYFUNCTIONAL ESTERS** | | | | | | | | | | | |
| METHYL SALICYLATE | 119-36-8 | 101 | 6.3814E+00 | -8.3884E+03 | 0 | 1.1532E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| 2-ETHOXYETHYL ACETATE | 111-15-9 | 101 | -7.8319E+00 | 1.3675E+03 | 0 | 0 | 0 | 273.15 | 363.15 | < 5% | E |
| ETHYL ACETOACETATE | 141-97-9 | 101 | -6.1053E+00 | 5.8199E+02 | 0 | 0 | 0 | 273.15 | 303.15 | < 25% | E |
| ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 112-07-2 | 101 | 1.0526E+01 | -1.1809E+04 | 0 | 2.0227E+06 | -2 | 273.15 | 363.35 | < 25% | E |
| **POLYOLS** | | | | | | | | | | | |
| p-HYDROQUINONE | 123-31-9 | 101 | 3.4838E+01 | -2.0077E+04 | 0 | 2.4975E+06 | -2 | 280.5 | 342.1 | < 3% | E |
| XYLITOL | 87-99-0 | 101 | 6.3503E+00 | -2.4082E+03 | 0 | 0 | 0 | 293.28 | 328.21 | < 5% | E |
| 1,3-BENZENEDIOL | 108-46-3 | 101 | 5.3815E+00 | -2.0610E+03 | 0 | 0 | 0 | 298.15 | 382.55 | < 3% | E |
| **PROPIONATES AND BUTYRATES** | | | | | | | | | | | |
| METHYL PROPIONATE | 554-12-1 | 101 | -5.4523E-01 | -3.0228E+03 | 0 | 5.6240E+05 | -2 | 273.15 | 343.35 | < 3% | E |
| ETHYL PROPIONATE | 105-37-3 | 101 | 8.6870E+00 | -9.6576E+03 | 0 | 1.6020E+06 | -2 | 273.15 | 353.45 | < 25% | E |
| n-PROPYL PROPIONATE | 106-36-5 | 101 | 2.3221E+00 | -6.9160E+03 | 0 | 1.2331E+06 | -2 | 273.15 | 363.65 | < 10% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| n-BUTYL PROPIONATE | 590-01-2 | 101 | 4.6182E+00 | -8.9538E+03 | 0 | 1.5193E+06 | -2 | 273.15 | 363.55 | < 5% | E |
| n-PROPYL n-BUTYRATE | 105-66-8 | 101 | 4.9548E+00 | -8.9029E+03 | 0 | 1.4776E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| METHYL n-BUTYRATE | 623-42-7 | 101 | 2.4057E+00 | -5.8594E+03 | 0 | 1.0181E+06 | -2 | 273.15 | 363.65 | < 25% | E |
| ETHYL n-BUTYRATE | 105-54-4 | 101 | -1.0853E-01 | -5.2994E+03 | 0 | 9.7757E+05 | -2 | 273.15 | 363.65 | < 25% | E |
| ISOBUTYL ISOBUTYRATE | 97-85-8 | 101 | 3.3149E+00 | -8.8385E+03 | 0 | 1.4943E+06 | -2 | 273.15 | 363.45 | < 25% | E |
| n-BUTYL n-BUTYRATE | 109-21-7 | 101 | 8.5669E+00 | -1.2335E+04 | 0 | 2.0772E+06 | -2 | 273.15 | 363.45 | < 10% | E |
| METHYL ISOBUTYRATE | 547-63-7 | 101 | 1.6346E+00 | -5.4561E+03 | 0 | 9.7055E+05 | -2 | 273.15 | 353.45 | < 3% | E |
| ETHYL ISOBUTYRATE | 97-62-1 | 101 | -2.9548E-01 | -5.2398E+03 | 0 | 9.7076E+05 | -2 | 273.15 | 363.75 | < 10% | E |
| n-PENTYL n-BUTYRATE | 540-18-1 | 101 | -1.1103E+01 | 2.1889E+02 | 0 | 0 | 0 | 273.15 | 363.65 | < 25% | E |
| ISOPENTYL BUTYRATE | 106-27-4 | 101 | 4.3536E+00 | -1.0210E+04 | 0 | 1.7238E+06 | -2 | 282.55 | 363.85 | < 100% | E |
| **SULFIDES/THIOPHENES** | | | | | | | | | | | |
| DIMETHYL SULFIDE | 75-18-3 | 101 | 6.9652E+00 | -7.2665E+03 | 0 | 1.0944E+06 | -2 | 272.35 | 353.45 | < 25% | EP |
| DIMETHYL DISULFIDE | 624-92-0 | 101 | -4.5077E+00 | -8.8322E+02 | 0 | 0 | 0 | 273.2 | 343.15 | < 10% | P |
| 2-METHYLTHIOPHENE | 554-14-3 | 101 | -7.2777E+00 | -3.1058E+02 | 0 | 0 | 0 | 298.15 | 343.15 | < 10% | E |
| DIISOPROPYL SULFIDE | 625-80-9 | 101 | -1.2690E+01 | 2.1122E+03 | 0 | -2.9537E+05 | -2 | 298.15 | 343.15 | < 25% | E |
| **UNSATURATED ALIPHATIC ESTERS** | | | | | | | | | | | |
| ETHYL ACRYLATE | 140-88-5 | 101 | 1.0372E+00 | -4.1664E+03 | 0 | 6.4977E+05 | -2 | 298.6 | 360.2 | < 10% | E |
| METHYL METHACRYLATE | 80-62-6 | 101 | 7.2435E+00 | -8.2103E+03 | 0 | 1.2803E+06 | -2 | 273.15 | 353.15 | < 5% | E |

Table C.4: $x_i^{aq}$ regression summary (cont.)

| Name | CAS | Eq | A | B | C | D | E | Tmin | Tmax | s | DT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DIETHYL MALEATE | 141-05-9 | 101 | 7.0429E+00 | -8.5650E+03 | 0 | 1.3541E+06 | -2 | 273.15 | 364.05 | < 5% | E |
| DIMETHYL MALEATE | 624-48-6 | 101 | 3.5518E+00 | -4.5854E+03 | 0 | 6.4474E+05 | -2 | 273.15 | 363.65 | < 3% | E |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| **1-ALKENES** | | | | | | | | | | |
| 1-PENTENE | 109-67-1 | 4.5386E-05 | < 25% | S | 1.8667E+06 | < 25% | S | 2.2033E+04 | < 25% | S |
| 1-HEXENE | 592-41-6 | 1.0983E-05 | < 10% | S | 2.1902E+06 | < 25% | S | 9.1053E+04 | < 10% | S |
| 1-HEXENE | 592-41-6 | 1.0983E-05 | < 10% | S | 2.1902E+06 | < 25% | S | 9.1053E+04 | < 10% | S |
| 1-HEPTENE | 592-76-7 | 2.6578E-06 | < 10% | S | 2.8281E+06 | < 10% | S | 3.7625E+05 | < 10% | S |
| 1-OCTENE | 111-66-0 | 6.4314E-07 | < 10% | S | 3.5550E+06 | < 10% | S | 1.5549E+06 | < 10% | S |
| 1-NONENE | 124-11-8 | 1.5564E-07 | < 25% | S | 4.8537E+06 | < 25% | S | 6.4250E+06 | < 25% | S |
| 1-DECENE | 872-05-9 | 3.7663E-08 | < 25% | P | 6.4586E+06 | < 25% | P | 2.6552E+07 | < 25% | P |
| 1-DECENE | 872-05-9 | 3.7663E-08 | < 25% | P | 6.4586E+06 | < 25% | P | 2.6552E+07 | < 25% | P |
| 1-DECENE | 872-05-9 | 3.7663E-08 | < 25% | P | 6.4586E+06 | < 25% | P | 2.6552E+07 | < 25% | P |
| 1-DECENE | 872-05-9 | 3.7663E-08 | < 25% | P | 6.4586E+06 | < 25% | P | 2.6552E+07 | < 25% | P |
| 1-PENTADECENE | 13360-61-7 | 3.1253E-11 | < 50% | S | 2.4928E+07 | < 50% | S | 3.1997E+10 | < 50% | S |
| **2,3,4-ALKENES** | | | | | | | | | | |
| cis-2-PENTENE | 627-20-3 | 5.2143E-05 | < 5% | E | 1.2624E+06 | < 5% | D | 1.9178E+04 | < 5% | D |
| trans-2-PENTENE | 646-04-8 | 5.2143E-05 | < 5% | E | 1.2932E+06 | < 5% | D | 1.9178E+04 | < 5% | D |
| cis-2-HEPTENE | 6443-92-1 | 2.7522E-06 | < 10% | E | 2.3412E+06 | < 10% | D | 3.6334E+05 | < 10% | D |
| trans-2-HEPTENE | 14686-13-6 | 2.7522E-06 | < 10% | E | 2.2918E+06 | < 10% | D | 3.6334E+05 | < 10% | D |
| **ACETATES** | | | | | | | | | | |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| METHYL ACETATE | 79-20-9 | 6.9553E-02 | < 3% | S | 6.7019E+02 | < 10% | S | 2.3439E+01 | < 10% | S |
| ETHYL ACETATE | 141-78-6 | 1.6041E-02 | < 3% | S | 8.4064E+02 | < 10% | S | 6.7660E+01 | < 10% | S |
| n-PROPYL ACETATE | 109-60-4 | 3.7965E-03 | < 5% | S | 1.2278E+03 | < 10% | S | 2.7549E+02 | < 10% | S |
| n-BUTYL ACETATE | 123-86-4 | 1.0141E-03 | < 10% | S | 1.4682E+03 | < 10% | S | 9.8461E+02 | < 10% | S |
| ISOBUTYL ACETATE | 110-19-0 | 1.0669E-03 | < 10% | S | 2.1658E+03 | < 10% | S | 9.1034E+02 | < 10% | S |
| ISOPENTYL ACETATE | 123-92-2 | 2.9009E-04 | < 10% | S | 2.7926E+03 | < 10% | S | 3.4340E+03 | < 10% | S |
| ISOPROPYL ACETATE | 108-21-4 | 4.7173E-03 | < 10% | S | 1.6585E+03 | < 25% | S | 2.0593E+02 | < 25% | S |
| sec-BUTYL ACETATE | 105-46-4 | 1.2134E-03 | < 10% | S | 2.4256E+03 | < 10% | S | 8.1913E+02 | < 10% | S |
| VINYL ACETATE | 108-05-4 | 5.4579E-03 | < 3% | S | 2.7687E+03 | < 3% | S | 1.8316E+02 | < 10% | S |
| n-PENTYL ACETATE | 628-63-7 | 2.5034E-04 | < 10% | S | 2.2402E+03 | < 10% | S | 3.9828E+03 | < 10% | S |
| n-HEXYL ACETATE | 142-92-7 | 5.9728E-05 | < 25% | S | 2.9135E+03 | < 25% | S | 1.6595E+04 | < 25% | S |
| n-HEPTYL ACETATE | 112-06-1 | 1.5184E-05 | < 25% | P | 3.8109E+03 | < 25% | P | 6.5861E+04 | < 25% | P |
| n-OCTYL ACETATE | 112-14-1 | 3.7799E-06 | < 25% | P | 5.4713E+03 | < 25% | P | 2.6455E+05 | < 25% | P |
| ETHYLENE GLYCOL DIACETATE | 111-55-7 | 2.3492E-02 | < 3% | S | - | - | - | - | - | - |
| tert-BUTYL ACETATE | 540-88-5 | 1.1407E-03 | < 3% | S | 4.7259E+03 | < 3% | S | 8.7411E+02 | < 10% | S |
| CYCLOHEXYL ACETATE | 622-45-7 | 3.4601E-04 | < 10% | S | 5.0496E+02 | < 10% | S | 2.8802E+03 | < 25% | S |
| PHENYL ACETATE | 122-79-2 | 7.6266E-04 | < 5% | S | 4.2332E+01 | < 5% | S | 1.3057E+03 | < 25% | S |
| **ALDEHYDES** | | | | | | | | | | |
| ACETALDEHYDE | 75-07-0 | 2.6796E-01 | < 10% | P | 3.7813E+02 | < 10% | S | - | - | - |
| PROPANAL | 123-38-6 | 1.2435E-01 | < 25% | S | 4.3628E+02 | < 5% | S | 1.0275E+01 | < 5% | S |
| BUTANAL | 123-72-8 | 1.7165E-02 | < 10% | S | 6.0597E+02 | < 5% | S | 4.0709E+01 | < 10% | S |
| 2-METHYLPROPANAL | 78-84-2 | 1.3236E-02 | < 3% | S | 1.0934E+03 | < 5% | S | 5.1912E+01 | < 5% | S |
| PENTANAL | 110-62-3 | 3.7043E-03 | < 25% | S | 8.3509E+02 | < 5% | S | 1.8344E+02 | < 10% | S |
| HEPTANAL | 111-71-7 | 2.3651E-04 | < 10% | S | 1.6308E+03 | < 10% | S | 3.1958E+03 | < 25% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| HEXANAL | 66-25-1 | 8.5071E-04 | < 25% | S | 1.2229E+03 | < 25% | S | 8.4624E+02 | < 25% | S |
| OCTANAL | 124-13-0 | 6.2433E-05 | < 50% | S | 2.7045E+03 | < 10% | S | 1.7662E+04 | < 25% | S |
| NONANAL | 124-19-6 | 7.2257E-06 | < 50% | S | 4.9990E+03 | < 25% | S | 1.3820E+05 | < 25% | S |
| 2-ETHYLHEXANAL | 123-05-7 | 5.6992E-05 | < 25% | S | 4.7357E+03 | < 25% | S | 1.7457E+04 | < 25% | S |
| 2-ETHYL-2-HEXENAL | 645-62-5 | 1.7449E-04 | < 25% | S | 1.0617E+03 | < 50% | S | 5.6988E+03 | < 50% | S |
| DECANAL | 112-31-2 | 1.4607E-06 | < 50% | S | 8.7393E+03 | < 100% | S | 6.8367E+05 | < 100% | S |
| 2-METHYLBUTYRALDEHYDE | 96-17-3 | 3.2304E-03 | < 10% | S | 2.2328E+03 | < 25% | P | 3.0863E+02 | < 25% | P |
| ACROLEIN | 107-02-8 | 8.6576E-02 | < 10% | S | 7.6218E+02 | < 100% | E | 2.0967E+01 | > 100% | S |
| trans-CROTONALDEHYDE | 123-73-9 | 4.6146E-02 | < 10% | S | 1.0285E+02 | < 25% | S | 2.1898E+01 | < 25% | S |
| METHACROLEIN | 78-85-3 | 1.6226E-02 | < 10% | S | 1.2347E+03 | < 10% | S | 6.1659E+01 | < 10% | S |
| p-TOLUALDEHYDE | 104-87-0 | 2.7792E-04 | < 10% | S | 1.0440E+02 | < 50% | S | 2.4875E+03 | < 50% | S |
| BENZALDEHYDE | 100-52-7 | 1.1842E-03 | < 10% | S | 1.4523E+02 | < 10% | S | 8.5631E+02 | < 10% | S |
| m-TOLUALDEHYDE | 620-23-5 | - | - | - | 1.6029E+02 | < 25% | S | 3.5526E+03 | < 50% | S |
| **ALIPHATIC ETHERS** | | | | | | | | | | |
| DIETHYL ETHER | 60-29-7 | 1.5055E-02 | < 3% | S | 5.7579E+03 | < 3% | S | 8.0282E+01 | < 5% | S |
| DIISOPROPYL ETHER | 108-20-3 | 1.6091E-03 | < 10% | S | 1.2343E+04 | < 10% | S | 6.2256E+02 | < 10% | S |
| DI-n-BUTYL ETHER | 142-96-1 | 3.1637E-05 | < 25% | S | 2.6272E+04 | < 25% | S | 3.1840E+04 | < 25% | S |
| METHYL tert-BUTYL ETHER | 1634-04-4 | 8.0111E-03 | < 5% | S | 4.1832E+03 | < 5% | S | 1.2555E+02 | < 10% | S |
| METHYL ISOBUTYL ETHER | 625-44-5 | 2.2379E-03 | < 5% | S | 1.2742E+04 | < 10% | S | 4.4655E+02 | < 10% | S |
| DI-n-HEXYL ETHER | 112-58-3 | 6.8917E-08 | < 25% | P | 8.9153E+04 | < 25% | P | 1.4510E+07 | < 25% | P |
| METHYL n-BUTYL ETHER | 628-28-4 | 1.7201E-03 | < 25% | S | 1.0077E+04 | < 25% | S | 5.5095E+02 | < 25% | S |
| DI-n-PENTYL ETHER | 693-65-2 | 2.2173E-06 | < 25% | P | 5.1508E+04 | < 25% | P | 4.5100E+05 | < 25% | P |
| METHYL tert-PENTYL ETHER | 994-05-8 | 1.7852E-03 | < 10% | S | 5.6708E+03 | < 10% | S | 5.6458E+02 | < 10% | S |
| tert-BUTYL ETHYL ETHER | 637-92-3 | 2.6488E-03 | < 25% | S | 7.7653E+03 | < 10% | S | 4.6299E+02 | < 25% | S |
| ETHYL tert-PENTYL ETHER | 919-94-8 | 4.9313E-04 | < 25% | S | 1.1017E+04 | < 25% | S | 2.0257E+03 | < 25% | S |

## Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| DI-n-PROPYL ETHER | 111-43-3 | 4.5240E-04 | < 5% | S | 1.8369E+04 | < 5% | S | 2.2134E+03 | < 10% | S |
| n-BUTYL ETHYL ETHER | 628-81-9 | 1.0019E-03 | < 25% | S | 7.2904E+03 | < 25% | S | 9.9042E+02 | < 25% | S |
| **ALKYLCYCLOHEXANES** | | | | | | | | | | |
| METHYLCYCLOHEXANE | 108-87-2 | 2.8767E-06 | < 25% | S | 2.1421E+06 | < 25% | S | 3.4764E+05 | < 25% | S |
| ETHYLCYCLOHEXANE | 1678-91-7 | 6.1015E-07 | < 5% | S | 2.7811E+06 | < 10% | S | 1.6267E+06 | < 10% | S |
| cis-1,2-DIMETHYLCYCLOHEXANE | 2207-01-4 | 9.5855E-07 | < 3% | S | 2.0121E+06 | < 10% | S | 1.0422E+06 | < 25% | S |
| trans-1,2-DIMETHYLCYCLOHEXANE | 6876-23-9 | 7.4961E-07 | < 3% | S | 3.4285E+06 | < 5% | S | 1.3281E+06 | < 5% | S |
| **ALKYLCYCLOPENTANES** | | | | | | | | | | |
| METHYLCYCLOPENTANE | 96-37-7 | 9.1506E-06 | < 3% | S | 2.0047E+06 | < 3% | S | 1.0935E+05 | < 3% | S |
| **ALKYNES** | | | | | | | | | | |
| ETHYLACETYLENE | 107-00-6 | 1.0280E-03 | < 25% | S | 9.8530E+04 | < 25% | S | - | - | - |
| 1-PENTYNE | 627-19-0 | 4.0450E-04 | < 25% | S | 1.4360E+05 | < 25% | S | 2.4720E+03 | < 25% | S |
| 1-HEXYNE | 693-02-7 | 8.4660E-05 | < 25% | S | 2.0930E+05 | < 25% | S | 1.1810E+04 | < 25% | S |
| 1-OCTYNE | 629-05-0 | 3.9470E-06 | < 25% | S | 4.4450E+05 | < 25% | S | 2.5340E+05 | < 25% | S |
| 1-NONYNE | 3452-09-3 | 7.6320E-07 | < 25% | S | 6.4770E+05 | < 25% | S | 1.3100E+06 | < 25% | S |
| 1-HEPTYNE | 628-71-7 | 1.8240E-05 | < 25% | S | 3.0500E+05 | < 25% | S | 5.4810E+04 | < 25% | S |
| **AROMATIC ALCOHOLS** | | | | | | | | | | |
| 2,3-XYLENOL | 526-75-0 | 6.9753E-04 | < 50% | S | - | - | - | - | - | - |
| 2,4-XYLENOL | 105-67-9 | 1.2252E-03 | < 25% | S | 1.5966E+01 | > 100% | S | 9.0061E+02 | > 100% | S |
| 2,5-XYLENOL | 95-87-4 | 5.1962E-04 | < 25% | S | 7.0922E+00 | < 25% | S | 4.7001E+02 | < 25% | S |
| 2,6-XYLENOL | 576-26-1 | 9.1715E-04 | < 50% | S | 3.4833E+01 | < 10% | S | 8.9965E+02 | < 25% | S |
| 3,4-XYLENOL | 95-65-8 | 8.5953E-04 | < 25% | S | 2.1606E+00 | < 25% | S | 4.9566E+02 | < 50% | S |
| 3,5-XYLENOL | 108-68-9 | 7.8450E-04 | < 25% | S | 3.5323E+00 | < 25% | S | 6.0576E+02 | < 25% | S |
| BENZYL ALCOHOL | 100-51-6 | 7.5540E-03 | < 5% | S | - | - | - | - | - | - |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| PHENOL | 108-95-2 | 1.6095E-02 | < 10% | S | 2.5082E+00 | < 25% | S | 4.3116E+01 | < 25% | S |
| o-CRESOL | 95-48-7 | 4.4173E-03 | < 25% | S | 8.2552E+00 | < 5% | S | 1.9993E+02 | < 10% | S |
| m-CRESOL | 108-39-4 | 3.8787E-03 | < 10% | S | 4.8030E+00 | < 25% | S | 2.5942E+02 | < 25% | S |
| p-CRESOL | 106-44-5 | 3.2357E-03 | < 10% | S | 4.3850E+00 | < 3% | S | 2.4356E+02 | < 10% | S |
| p-ETHYLPHENOL | 123-07-9 | 1.0065E-03 | < 100% | S | - | - | - | - | - | - |
| 2-PHENYLETHANOL | 60-12-8 | 3.6435E-03 | < 10% | S | 3.1574E+00 | < 10% | P | 2.7319E+02 | < 25% | P |
| 1-PHENYL-1-PROPANOL | 93-54-9 | 1.3678E-03 | < 5% | S | - | - | - | - | - | - |
| **AROMATIC AMINES** | | | | | | | | | | |
| o-TOLUIDINE | 95-53-4 | 3.0033E-03 | < 25% | S | 1.1565E+01 | < 25% | S | 3.3124E+02 | < 25% | S |
| m-TOLUIDINE | 108-44-1 | 2.6391E-03 | < 25% | S | 9.8018E+00 | < 25% | S | 3.7689E+02 | < 25% | S |
| p-TOLUIDINE | 106-49-0 | 1.4028E-03 | < 3% | S | 1.9157E+01 | < 3% | S | 4.5491E+02 | < 50% | S |
| QUINOLINE | 91-22-5 | 1.0010E-03 | < 25% | S | - | - | - | - | - | - |
| N,N-DIETHYLANILINE | 91-66-7 | 2.1975E-05 | < 5% | S | 8.3101E+02 | < 10% | S | 4.4708E+04 | < 25% | S |
| PYRIDINE | 110-86-1 | 1.0000E+00 | Unknown | E | 6.1142E+01 | < 25% | S | 2.1558E+01 | < 25% | S |
| ANILINE | 62-53-3 | 7.2058E-03 | < 3% | S | 1.1727E+01 | < 10% | S | 1.3007E+02 | < 10% | S |
| 2-METHYLPYRIDINE | 109-06-8 | 1.0000E+00 | Unknown | E | 5.6453E+01 | < 5% | S | 3.7361E+01 | < 5% | S |
| o-ETHYLANILINE | 578-54-1 | 1.0298E-03 | < 10% | S | 2.2524E+01 | < 10% | P | 9.6769E+02 | < 25% | P |
| DIBENZOPYRROLE | 86-74-8 | - | - | - | 5.9192E-01 | < 50% | S | - | - | - |
| 2,4,6-TRIMETHYLPYRIDINE | 108-75-8 | 4.4755E-03 | < 25% | S | - | - | - | - | - | - |
| 2,6-DIMETHYLPYRIDINE | 108-48-5 | 1.0000E+00 | Unknown | E | 6.0121E+01 | < 25% | S | 7.7723E+01 | < 25% | S |
| 3-METHYLPYRIDINE | 108-99-6 | 1.0000E+00 | Unknown | E | 4.4215E+01 | < 25% | S | 5.4547E+01 | < 25% | S |
| 4-METHYLPYRIDINE | 108-89-4 | 1.0000E+00 | Unknown | E | 3.3943E+01 | < 5% | S | 4.4159E+01 | < 5% | S |
| 2,4-DIMETHYLANILINE | 95-68-1 | 8.1102E-04 | < 10% | S | 2.0392E+01 | < 25% | P | 1.2231E+03 | < 50% | P |
| N-ETHYLANILINE | 103-69-5 | 3.9949E-04 | < 3% | S | 6.5222E+01 | < 10% | S | 2.4020E+03 | < 25% | S |
| **AROMATIC CARBOXYLIC ACIDS** | | | | | | | | | | |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| o-TOLUIC ACID | 118-90-1 | 1.5612E-04 | < 25% | S | - | - | - | - | - | - |
| p-TOLUIC ACID | 99-94-5 | 4.6846E-05 | < 5% | S | - | - | - | - | - | - |
| PHTHALIC ACID | 88-99-3 | 6.9289E-04 | < 5% | S | - | - | - | - | - | - |
| m-TOLUIC ACID | 99-04-7 | 1.1411E-04 | < 3% | S | - | - | - | - | - | - |
| **AROMATIC CHLORIDES** | | | | | | | | | | |
| BENZYL CHLORIDE | 100-44-7 | 6.9223E-05 | < 25% | S | 2.5098E+03 | < 25% | S | 1.4426E+04 | < 25% | S |
| MONOCHLOROBENZENE | 108-90-7 | 7.3850E-05 | < 5% | S | 2.1129E+04 | < 5% | S | 1.3325E+04 | < 10% | S |
| o-DICHLOROBENZENE | 95-50-1 | 1.7571E-05 | < 10% | S | 1.0267E+04 | < 10% | S | 5.6832E+04 | < 10% | S |
| m-DICHLOROBENZENE | 541-73-1 | 1.5956E-05 | < 10% | S | 1.7908E+04 | < 10% | S | 6.2774E+04 | < 10% | S |
| p-DICHLOROBENZENE | 106-46-7 | 9.8562E-06 | < 10% | S | 1.3908E+04 | < 10% | S | 5.5428E+04 | < 10% | S |
| HEXACHLOROBENZENE | 118-74-1 | 3.6635E-10 | < 25% | S | 8.4566E+03 | < 25% | S | 1.8179E+08 | < 100% | S |
| o-CHLOROTOLUENE | 95-49-8 | 1.8949E-05 | < 25% | S | 2.4693E+04 | < 25% | S | 5.2836E+04 | < 25% | S |
| p-CHLOROTOLUENE | 106-43-4 | 1.7936E-05 | < 25% | S | 2.0445E+04 | < 25% | S | 5.5321E+04 | < 25% | S |
| 2,4-DICHLOROTOLUENE | 95-73-8 | 2.9825E-06 | < 5% | S | 2.0337E+04 | < 5% | S | 3.3512E+05 | < 10% | S |
| 1,2,4-TRICHLOROBENZENE | 120-82-1 | 4.0753E-06 | < 25% | S | 1.3112E+04 | < 25% | S | 2.5357E+05 | < 25% | S |
| 1,2,3-TRICHLOROBENZENE | 87-61-6 | 2.0122E-06 | < 10% | S | 8.9256E+03 | < 10% | S | 2.9730E+05 | < 25% | S |
| **AROMATIC ESTERS** | | | | | | | | | | |
| BENZYL ACETATE | 140-11-4 | 3.0871E-04 | < 5% | S | 6.5097E+01 | < 10% | S | 3.1178E+03 | < 25% | S |
| DI-n-PROPYL PHTHALATE | 131-16-8 | 6.6314E-06 | < 25% | S | 2.5555E+00 | < 25% | S | 1.5080E+05 | < 25% | S |
| DI-n-HEXYL PHTHALATE | 84-75-3 | 1.2643E-08 | < 50% | S | 6.6872E+00 | < 50% | S | 7.9098E+07 | < 50% | S |
| METHYL BENZOATE | 93-58-3 | 2.7549E-04 | < 25% | S | 1.8175E+02 | < 25% | S | 3.6117E+03 | < 25% | S |
| ETHYL BENZOATE | 93-89-0 | 1.1434E-04 | < 25% | S | 3.3110E+02 | < 25% | S | 8.7005E+03 | < 25% | S |
| BENZYL FORMATE | 104-57-4 | 1.2812E-03 | < 25% | S | 2.8015E+01 | < 10% | S | 6.8470E+02 | < 25% | S |
| DIETHYL PHTHALATE | 84-66-2 | 7.5610E-05 | < 10% | S | 8.9347E-01 | < 5% | S | 1.3457E+04 | < 25% | S |
| DI-n-BUTYL PHTHALATE | 84-74-2 | 6.4443E-07 | < 25% | S | 5.2831E+00 | < 25% | S | 1.5514E+06 | < 25% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| DIMETHYL PHTHALATE | 131-11-3 | 4.1370E-04 | < 5% | S | 1.1053E+00 | < 5% | P | 2.4220E+03 | < 25% | P |
| **C, H, BR COMPOUNDS** | | | | | | | | | | |
| BROMOMETHANE | 74-83-9 | 2.6893E-03 | < 25% | S | 3.7821E+04 | < 25% | S | - | - | - |
| BROMOETHANE | 74-96-4 | 1.5050E-03 | < 3% | S | 4.1374E+04 | < 3% | S | 6.6333E+02 | < 10% | S |
| 1,1,2,2-TETRABROMOETHANE | 79-27-6 | 1.5750E-06 | < 50% | S | 3.8812E+03 | < 100% | S | 6.3403E+05 | < 100% | S |
| 1-BROMOPROPANE | 106-94-5 | 3.5257E-04 | < 3% | S | 5.2435E+04 | < 3% | S | 2.8283E+03 | < 5% | S |
| 2-BROMOPROPANE | 75-26-3 | 4.6986E-04 | < 3% | S | 6.1437E+04 | < 3% | S | 2.1294E+03 | < 5% | S |
| 1-BROMOBUTANE | 109-65-9 | 7.4063E-05 | < 25% | S | 7.4474E+04 | < 25% | S | 1.3502E+04 | < 25% | S |
| 1-BROMOHEPTANE | 629-04-9 | 7.4417E-07 | < 25% | S | 2.4825E+05 | < 25% | S | 1.3438E+06 | < 25% | S |
| 1,2-DIBROMOETHANE | 106-93-4 | 4.2706E-04 | < 10% | S | 4.0636E+03 | < 10% | S | 2.3308E+03 | < 10% | S |
| m-DIBROMOBENZENE | 108-36-1 | 7.5328E-06 | < 25% | E | 4.7500E+03 | < 25% | D | 1.3275E+05 | < 25% | D |
| BROMOBENZENE | 108-86-1 | 4.5894E-05 | < 5% | S | 1.2337E+04 | < 5% | S | 2.1731E+04 | < 10% | S |
| TRIBROMOMETHANE | 75-25-2 | 2.4116E-04 | < 5% | S | 3.0319E+03 | < 10% | S | 4.1402E+03 | < 10% | S |
| DIBROMOMETHANE | 74-95-3 | 1.2397E-03 | < 3% | S | 4.8569E+03 | < 3% | S | 8.0641E+02 | < 5% | S |
| 2-BROMOBUTANE | 78-76-2 | 1.2019E-04 | < 10% | D | 6.3195E+04 | < 10% | D | 8.3200E+03 | < 10% | E |
| p-BROMOTOLUENE | 106-38-7 | 1.1174E-05 | < 25% | S | 1.5321E+04 | < 25% | S | 8.4309E+04 | < 50% | S |
| **C, H, F COMPOUNDS** | | | | | | | | | | |
| METHYL FLUORIDE | 593-53-3 | 1.0604E-03 | < 1% | S | 9.5359E+04 | < 3% | S | - | - | - |
| PERFLUORO-n-HEXANE | 355-42-0 | 4.8787E-09 | < 100% | E | 5.9661E+09 | < 100% | D | 2.0497E+08 | < 100% | D |
| PERFLUORO-n-OCTANE | 307-34-6 | 6.8663E-11 | < 100% | E | 6.8797E+10 | < 100% | D | 1.4564E+10 | < 100% | D |
| 1,2-DIFLUOROBENZENE | 367-11-3 | 1.6957E-04 | < 25% | S | 4.2141E+04 | < 25% | S | 5.8883E+03 | < 25% | S |
| FLUOROBENZENE | 462-06-6 | 2.7647E-04 | < 10% | S | 3.7174E+04 | < 10% | S | 3.6155E+03 | < 10% | S |
| HEXAFLUOROBENZENE | 392-56-3 | 6.0415E-05 | < 3% | S | 1.8597E+05 | < 3% | S | 1.6515E+04 | < 5% | S |
| PERFLUORO-n-PENTANE | 678-26-2 | 7.2276E-08 | < 100% | E | 1.2114E+09 | < 100% | D | 1.3835E+07 | < 100% | D |
| PERFLUORO-n-HEPTANE | 335-57-9 | 5.6014E-10 | < 100% | E | 1.8284E+10 | < 100% | D | 1.7852E+09 | < 100% | D |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| **C, H, I COMPOUNDS** | | | | | | | | | | |
| METHYL IODIDE | 74-88-4 | 1.8484E-03 | < 5% | S | 2.9424E+04 | < 5% | S | 5.4150E+02 | < 10% | S |
| ETHYL IODIDE | 75-03-6 | 4.6009E-04 | < 3% | S | 3.8621E+04 | < 3% | S | 2.1744E+03 | < 10% | S |
| n-PROPYL IODIDE | 107-08-4 | 1.0973E-04 | < 5% | S | 5.2297E+04 | < 5% | S | 9.0990E+03 | < 10% | S |
| ISOPROPYL IODIDE | 75-30-9 | 1.4480E-04 | < 10% | S | 6.5461E+04 | < 5% | S | 6.8884E+03 | < 10% | S |
| IODOBENZENE | 591-50-4 | 1.9110E-05 | < 10% | S | 7.3212E+03 | < 25% | S | 5.1681E+04 | < 25% | S |
| n-HEXYL IODIDE | 638-45-9 | 1.1954E-06 | < 25% | S | 1.6347E+05 | < 25% | S | 8.3652E+05 | < 25% | S |
| n-BUTYL IODIDE | 542-69-8 | 2.2740E-05 | < 10% | S | 8.0572E+04 | < 25% | S | 4.3976E+04 | < 10% | S |
| **C, H, MULTIHALOGEN COMPOUNDS** | | | | | | | | | | |
| DICHLORODIFLUOROMETHANE | 75-71-8 | 5.4251E-05 | < 3% | S | 1.8669E+06 | < 10% | S | - | - | - |
| TRICHLOROFLUOROMETHANE | 75-69-4 | - | - | - | 5.2851E+05 | < 10% | S | - | - | - |
| 1,1,2-TRICHLOROTRIFLUOROETHANE | 76-13-1 | 2.3783E-05 | < 25% | S | 1.8719E+06 | < 25% | S | 4.2032E+04 | < 25% | S |
| **C, H, NO2 COMPOUNDS** | | | | | | | | | | |
| NITROMETHANE | 75-52-5 | 3.2090E-02 | < 10% | S | 1.4923E+02 | < 10% | S | 3.1049E+01 | < 10% | S |
| NITROETHANE | 79-24-3 | 1.0659E-02 | < 5% | S | 2.5784E+02 | < 5% | S | 9.3542E+01 | < 10% | S |
| 1-NITROPROPANE | 108-03-2 | 3.2369E-03 | < 5% | S | 4.1378E+02 | < 5% | S | 3.0767E+02 | < 10% | S |
| 2-NITROPROPANE | 79-46-9 | 3.5066E-03 | < 5% | S | 6.5009E+02 | < 3% | S | 2.8516E+02 | < 10% | S |
| 1-NITROBUTANE | 627-05-4 | 6.5301E-04 | < 25% | S | 7.2451E+02 | < 25% | S | 1.5314E+03 | < 25% | S |
| o-NITROTOLUENE | 88-72-2 | 8.4414E-05 | < 5% | S | 2.3476E+02 | < 10% | S | 1.1833E+04 | < 10% | S |
| p-NITROTOLUENE | 99-99-0 | 4.6972E-05 | < 10% | S | 6.2304E+01 | < 10% | S | 1.2362E+04 | < 50% | S |
| m-NITROTOLUENE | 99-08-1 | 6.6378E-05 | < 5% | S | 2.0274E+02 | < 10% | S | 1.4420E+04 | < 25% | S |
| NITROBENZENE | 98-95-3 | 2.8289E-04 | < 5% | S | 1.1835E+02 | < 5% | S | 3.5294E+03 | < 10% | S |
| m-DINITROBENZENE | 99-65-0 | 5.7572E-05 | < 10% | S | - | - | - | - | - | - |
| p-DINITROBENZENE | 100-25-4 | 6.6100E-06 | < 3% | S | - | - | - | - | - | - |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 2,4-DINITROTOLUENE | 121-14-2 | 1.9749E-05 | < 5% | S | 1.4084E+00 | < 5% | S | 1.6382E+04 | < 25% | S |
| 2,6-DINITROTOLUENE | 606-20-2 | 2.0406E-05 | < 5% | S | 1.1571E+01 | < 3% | S | 2.3491E+04 | < 50% | S |
| 3,4-DINITROTOLUENE | 610-39-9 | 1.6997E-05 | < 5% | S | 1.6741E+00 | < 5% | S | 2.6088E+04 | < 50% | S |
| 2,4,6-TRINITROTOLUENE | 118-96-7 | 9.5510E-06 | < 5% | S | 1.2083E-01 | < 5% | S | 2.1202E+04 | < 50% | S |
| RDX | 121-82-4 | 3.9683E-06 | < 5% | S | - | - | - | - | - | - |
| HMX | 2691-41-0 | 2.7726E-07 | < 10% | S | - | - | - | - | - | - |
| **C1/C2 ALIPHATIC CHLORIDES** | | | | | | | | | | |
| CARBON TETRACHLORIDE | 56-23-5 | 9.0660E-05 | < 5% | S | 1.6765E+05 | < 5% | S | 1.1029E+04 | < 5% | S |
| METHYL CHLORIDE | 74-87-3 | 1.9096E-03 | < 10% | S | 5.2937E+04 | < 10% | S | - | - | - |
| ETHYL CHLORIDE | 75-00-3 | 1.5332E-03 | < 25% | S | 6.6090E+04 | < 10% | S | - | - | - |
| VINYL CHLORIDE | 75-01-4 | 7.7389E-04 | < 25% | S | 1.3062E+05 | < 25% | S | - | - | - |
| DICHLOROMETHANE | 75-09-2 | 4.0143E-03 | < 10% | S | 1.4546E+04 | < 10% | S | 2.4938E+02 | < 10% | S |
| CHLOROFORM | 67-66-3 | 1.1812E-03 | < 3% | S | 2.2108E+04 | < 3% | S | 8.4620E+02 | < 5% | S |
| 1,1-DICHLOROETHANE | 75-34-3 | 9.3878E-04 | < 5% | S | 3.2146E+04 | < 5% | S | 1.0626E+03 | < 5% | S |
| 1,2-DICHLOROETHANE | 107-06-2 | 1.5990E-03 | < 5% | S | 6.6406E+03 | < 5% | S | 6.2532E+02 | < 5% | S |
| 1,1,2-TRICHLOROETHANE | 79-00-5 | 6.2690E-04 | < 5% | S | 4.9329E+03 | < 5% | S | 1.5984E+03 | < 5% | S |
| HEXACHLOROETHANE | 67-72-1 | 2.9288E-06 | < 25% | S | 2.0130E+04 | < 25% | S | 1.6173E+05 | > 100% | S |
| 1,1,1-TRICHLOROETHANE | 71-55-6 | 1.7505E-04 | < 5% | S | 9.4916E+04 | < 5% | S | 5.7096E+03 | < 10% | S |
| 1,1,1,2-TETRACHLOROETHANE | 630-20-6 | 1.1099E-04 | < 10% | S | 1.3082E+04 | < 10% | S | 8.2197E+03 | < 10% | S |
| 1,1,2,2-TETRACHLOROETHANE | 79-34-5 | 3.1284E-04 | < 10% | S | 2.3451E+03 | < 10% | S | 3.0753E+03 | < 10% | S |
| TRICHLOROETHYLENE | 79-01-6 | 1.8045E-04 | < 3% | S | 5.4319E+04 | < 3% | S | 5.5283E+03 | < 5% | S |
| TETRACHLOROETHYLENE | 127-18-4 | 2.4977E-05 | < 5% | S | 9.8707E+04 | < 5% | S | 3.9944E+04 | < 10% | S |
| cis-1,2-DICHLOROETHYLENE | 156-59-2 | 1.1760E-03 | < 10% | S | 2.3105E+04 | < 10% | S | 8.4974E+02 | < 10% | S |
| trans-1,2-DICHLOROETHYLENE | 156-60-5 | 8.2754E-04 | < 10% | S | 5.3633E+04 | < 10% | S | 1.2109E+03 | < 10% | S |
| PENTACHLOROETHANE | 76-01-7 | 3.6884E-05 | < 25% | S | 1.3266E+04 | < 25% | S | 2.7105E+04 | < 25% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 1,1-DICHLOROETHYLENE | 75-35-4 | 4.6806E-04 | < 10% | S | 1.7069E+05 | < 10% | S | 2.1390E+03 | < 10% | S |
| **C3 & HIGHER ALIPHATIC CHLORIDES** | | | | | | | | | | |
| 1,4-DICHLOROBUTANE | 110-56-5 | 1.8176E-04 | < 25% | S | 2.7961E+03 | < 10% | S | 5.4994E+03 | < 25% | S |
| 1,5-DICHLOROPENTANE | 628-76-2 | 2.5038E-05 | < 100% | S | 5.3788E+03 | < 100% | S | 3.9925E+04 | < 100% | S |
| 1,2-DICHLOROPROPANE | 78-87-5 | 4.3120E-04 | < 5% | S | 1.6001E+04 | < 5% | S | 2.3227E+03 | < 10% | S |
| ISOPROPYL CHLORIDE | 75-29-6 | 7.1457E-04 | < 10% | S | 9.6129E+04 | < 5% | S | 1.3976E+03 | < 10% | S |
| 1,2,3-TRICHLOROPROPANE | 96-18-4 | 2.8896E-04 | < 25% | S | 1.6851E+03 | < 25% | S | 3.4614E+03 | < 25% | S |
| HEXACHLORO-1,3-BUTADIENE | 87-68-3 | 3.1189E-07 | < 50% | S | 9.8863E+04 | < 50% | S | 3.1995E+06 | < 50% | S |
| PROPYL CHLORIDE | 540-54-5 | 6.3068E-04 | < 10% | S | 7.2709E+04 | < 10% | S | 1.5838E+03 | < 10% | S |
| n-BUTYL CHLORIDE | 109-69-3 | 1.3685E-04 | < 10% | S | 9.8517E+04 | < 10% | S | 7.3035E+03 | < 10% | S |
| sec-BUTYL CHLORIDE | 78-86-4 | 1.5548E-04 | < 10% | S | 1.3477E+05 | < 10% | S | 6.4263E+03 | < 10% | S |
| 1-CHLOROPENTANE | 543-59-9 | 3.3579E-05 | < 5% | S | 1.2764E+05 | < 5% | S | 2.9802E+04 | < 5% | S |
| 1,3-DICHLOROPROPANE | 142-28-9 | 3.7373E-04 | < 25% | S | 4.7562E+03 | < 25% | S | 2.6752E+03 | < 25% | S |
| **CYCLOALIPHATIC ALCOHOLS** | | | | | | | | | | |
| CYCLOHEXANOL | 108-93-0 | 6.9303E-03 | < 5% | S | 1.2847E+01 | < 50% | S | 1.4416E+02 | < 50% | S |
| **CYCLOALKANES** | | | | | | | | | | |
| CYCLOPENTANE | 287-92-3 | 4.3311E-05 | < 10% | S | 9.8100E+05 | < 10% | S | 2.3099E+04 | < 10% | S |
| CYCLOHEXANE | 110-82-7 | 1.3004E-05 | < 10% | S | 9.4972E+05 | < 10% | S | 7.2858E+04 | < 10% | S |
| CYCLOHEPTANE | 291-64-5 | 3.5216E-06 | < 10% | P | 8.2667E+05 | < 10% | P | 2.8396E+05 | < 10% | P |
| CYCLOOCTANE | 292-64-8 | 9.7862E-07 | < 10% | S | 7.6345E+05 | < 10% | S | 1.0159E+06 | < 10% | S |
| **CYCLOALKENES** | | | | | | | | | | |
| CYCLOPENTENE | 142-29-0 | 1.7784E-04 | < 50% | S | 2.8372E+05 | < 50% | S | 5.6203E+03 | < 50% | S |
| CYCLOHEXENE | 110-83-8 | 6.2535E-05 | < 10% | S | 1.8948E+05 | < 10% | S | 1.5966E+04 | < 10% | S |
| CYCLOHEPTENE | 628-92-2 | 1.2363E-05 | < 10% | E | 2.7050E+05 | < 25% | D | 8.0884E+04 | < 10% | D |
| CYCLOOCTENE | 931-88-4 | 3.8290E-06 | < 3% | S | 2.6909E+05 | < 3% | S | 2.6479E+05 | < 3% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| **DIALKENES** | | | | | | | | | | |
| 1,4-CYCLOHEXADIENE | 628-41-1 | 2.0206E-04 | < 25% | S | 4.3001E+04 | < 25% | S | 4.9455E+03 | < 25% | S |
| **DICARBOXYLIC ACIDS** | | | | | | | | | | |
| ADIPIC ACID | 124-04-9 | 2.9884E-03 | < 3% | S | - | - | - | - | - | - |
| SUCCINIC ACID | 110-15-6 | 1.3056E-02 | < 3% | S | - | - | - | - | - | - |
| GLUTARIC ACID | 110-94-1 | 1.6229E-01 | < 3% | S | - | - | - | - | - | - |
| **DIMETHYLALKANES** | | | | | | | | | | |
| 2,2-DIMETHYLBUTANE | 75-83-2 | 4.4181E-06 | < 25% | S | 9.7812E+06 | < 25% | S | 2.2886E+05 | < 25% | S |
| 2,3-DIMETHYLBUTANE | 79-29-8 | 4.2380E-06 | < 25% | S | 7.1887E+06 | < 25% | S | 2.3026E+05 | < 25% | S |
| 2,4-DIMETHYLPENTANE | 108-08-7 | 7.3837E-07 | < 50% | S | 1.9367E+07 | < 50% | S | 1.4765E+06 | < 50% | S |
| 3,3-DIMETHYLPENTANE | 562-49-2 | 1.0612E-06 | < 25% | S | 1.0373E+07 | < 25% | S | 9.4075E+05 | < 25% | S |
| 2,2-DIMETHYLHEXANE | 590-73-8 | 2.0105E-07 | < 3% | S | 2.2630E+07 | < 5% | S | 4.9870E+06 | < 5% | S |
| 2,5-DIMETHYLHEXANE | 592-13-2 | 1.7933E-07 | < 3% | S | 2.2712E+07 | < 3% | S | 5.6221E+06 | < 5% | S |
| **DIPHENYL/POLYAROMATICS** | | | | | | | | | | |
| BIPHENYL | 92-52-4 | 8.2180E-07 | < 10% | S | 1.5402E+03 | < 10% | S | 4.5922E+05 | < 10% | S |
| **EPOXIDES** | | | | | | | | | | |
| 2-METHYLTETRAHYDROFURAN | 96-47-9 | 3.0305E-02 | < 5% | S | - | - | - | - | - | - |
| 1,4-DIOXANE | 123-91-1 | - | - | - | 2.9564E+01 | < 10% | S | 5.8161E+00 | < 10% | S |
| TRIOXANE | 110-88-3 | 4.3058E-02 | < 50% | S | - | - | - | - | - | - |
| TETRAHYDROPYRAN | 142-68-7 | 1.7361E-02 | < 3% | S | 6.7975E+02 | < 5% | S | 7.1786E+01 | < 5% | S |
| TETRAHYDROFURAN | 109-99-9 | - | - | - | 3.7471E+02 | < 10% | S | 1.7501E+01 | < 10% | S |
| DIBENZOFURAN | 132-64-9 | 5.4315E-07 | < 10% | S | 7.4383E+02 | < 10% | S | 5.2639E+05 | < 25% | S |
| **FORMATES** | | | | | | | | | | |
| METHYL FORMATE | 107-31-3 | - | - | - | 1.3237E+03 | < 10% | D | 1.7005E+01 | < 10% | S |
| ETHYL FORMATE | 109-94-4 | 2.0624E-02 | < 3% | S | 1.6926E+03 | < 25% | S | 5.1845E+01 | < 25% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| n-PROPYL FORMATE | 110-74-7 | 5.6073E-03 | < 5% | S | 1.8180E+03 | < 10% | S | 1.6754E+02 | < 10% | S |
| n-BUTYL FORMATE | 592-84-7 | 1.7728E-03 | < 25% | S | 2.1415E+03 | < 25% | P | 5.6349E+02 | < 25% | P |
| ISOBUTYL FORMATE | 542-55-2 | 1.5568E-03 | < 10% | S | 3.3686E+03 | < 10% | S | 6.1884E+02 | < 10% | P |
| n-PENTYL FORMATE | 638-49-3 | 3.8458E-04 | < 25% | S | 3.0716E+03 | < 25% | S | 2.5812E+03 | < 25% | S |
| tert-BUTYL FORMATE | 762-75-4 | 2.8541E-03 | < 5% | S | 3.8948E+03 | < 5% | S | 3.5011E+02 | < 25% | S |
| **KETONES** | | | | | | | | | | |
| ACETONE | 67-64-1 | - | - | - | 1.9892E+02 | < 5% | S | 6.4743E+00 | < 10% | S |
| METHYL ETHYL KETONE | 78-93-3 | 8.0636E-02 | < 3% | S | 3.0126E+02 | < 10% | S | 2.4485E+01 | < 10% | S |
| 3-PENTANONE | 96-22-0 | 1.0287E-02 | < 10% | S | 5.8894E+02 | < 5% | S | 9.7081E+01 | < 10% | S |
| METHYL ISOBUTYL KETONE | 108-10-1 | 3.2450E-03 | < 10% | S | 8.1503E+02 | < 10% | S | 3.0755E+02 | < 25% | S |
| 3-HEPTANONE | 106-35-4 | 7.1140E-04 | < 10% | S | 7.8587E+02 | < 10% | S | 1.3989E+03 | < 25% | S |
| 4-HEPTANONE | 123-19-3 | 6.5059E-04 | < 10% | S | 1.1765E+03 | < 10% | S | 1.5279E+03 | < 25% | S |
| 3-HEXANONE | 589-38-8 | 2.6395E-03 | < 25% | S | 7.0108E+02 | < 10% | S | 3.7866E+02 | < 10% | S |
| 2-PENTANONE | 107-87-9 | 1.1528E-02 | < 5% | S | 4.0969E+02 | < 5% | S | 8.6500E+01 | < 10% | S |
| METHYL ISOPROPYL KETONE | 563-80-4 | 1.3715E-02 | < 5% | S | 5.1455E+02 | < 5% | P | 7.4588E+01 | < 10% | P |
| 2-HEXANONE | 591-78-6 | 2.8457E-03 | < 5% | S | 5.4080E+02 | < 5% | S | 3.4847E+02 | < 10% | S |
| 2-HEPTANONE | 110-43-0 | 6.4445E-04 | < 3% | S | 8.0639E+02 | < 3% | S | 1.5469E+03 | < 5% | P |
| 5-METHYL-2-HEXANONE | 110-12-3 | 7.7380E-04 | < 5% | S | 8.8878E+02 | < 5% | S | 1.2828E+03 | < 5% | S |
| 3,3-DIMETHYL-2-BUTANONE | 75-97-8 | 3.4404E-03 | < 5% | S | 1.2372E+03 | < 5% | S | 2.8979E+02 | < 25% | S |
| DIISOBUTYL KETONE | 108-83-8 | 5.1396E-05 | < 10% | S | 4.3295E+03 | < 10% | S | 1.9301E+04 | < 10% | S |
| DIISOPROPYL KETONE | 565-80-0 | 7.8573E-04 | < 10% | S | 2.4265E+03 | < 10% | S | 1.2694E+03 | < 25% | S |
| 5-NONANONE | 502-56-7 | 5.6855E-05 | < 25% | S | 1.3894E+03 | < 25% | S | 1.7526E+04 | < 25% | S |
| 2-NONANONE | 821-55-6 | 4.2752E-05 | < 25% | S | 1.5963E+03 | < 25% | S | 2.3810E+04 | < 25% | S |
| ACETYLACETONE | 123-54-6 | 3.3792E-02 | < 5% | S | 6.4870E+01 | < 25% | S | 4.9594E+01 | < 50% | S |
| ISOPHORONE | 78-59-1 | 1.8712E-03 | < 3% | S | - | - | - | - | - | - |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| CYCLOPENTANONE | 120-92-3 | 8.0153E-02 | < 3% | S | 4.4727E+01 | < 100% | S | 2.9473E+01 | < 100% | S |
| CYCLOHEXANONE | 108-94-1 | 1.7464E-02 | < 5% | S | 3.6312E+01 | < 25% | S | 6.4858E+01 | < 25% | S |
| 2-OCTANONE | 111-13-7 | 1.8040E-04 | < 25% | S | 1.0319E+03 | < 25% | S | 5.5108E+03 | < 25% | S |
| ACETOPHENONE | 98-86-2 | 9.1777E-04 | < 25% | S | 5.0333E+01 | < 25% | S | 9.5225E+02 | < 25% | S |
| 3-OCTANONE | 106-68-3 | 1.8418E-04 | < 10% | S | 1.3047E+03 | < 10% | S | 5.4089E+03 | < 25% | S |
| 3-NONANONE | 925-78-0 | 6.3260E-05 | < 25% | S | 1.0827E+03 | < 25% | S | 1.5675E+04 | < 25% | S |
| 2,6,8-TRIMETHYL-4-NONANONE | 123-18-2 | 2.2065E-06 | < 25% | P | 5.2094E+03 | < 25% | P | 4.5321E+05 | < 25% | P |
| **MERCAPTANS** | | | | | | | | | | |
| ISOPROPYL MERCAPTAN | 75-33-2 | 8.7844E-04 | < 10% | S | 4.1922E+04 | < 10% | S | 1.1366E+03 | < 10% | S |
| n-BUTYL MERCAPTAN | 109-79-5 | 1.6284E-04 | < 3% | S | 3.7378E+04 | < 5% | S | 6.0435E+03 | < 10% | S |
| **METHYLALKANES** | | | | | | | | | | |
| 2-METHYLPENTANE | 107-83-5 | 3.0912E-06 | < 25% | S | 8.9514E+06 | < 10% | S | 3.1860E+05 | < 25% | S |
| 3-METHYLPENTANE | 96-14-0 | 2.7067E-06 | < 3% | S | 9.3257E+06 | < 3% | S | 3.6949E+05 | < 3% | S |
| 2-METHYLHEXANE | 591-76-4 | 4.5667E-07 | < 5% | E | 1.9204E+07 | < 10% | D | 2.1898E+06 | < 5% | D |
| 3-METHYLHEXANE | 589-34-4 | 4.7716E-07 | < 5% | S | 1.7157E+07 | < 10% | S | 2.0958E+06 | < 5% | S |
| 3-METHYLHEPTANE | 589-81-1 | 1.2491E-07 | < 5% | E | 2.0935E+07 | < 10% | S | 8.0059E+06 | < 10% | S |
| 4-METHYLHEPTANE | 589-53-7 | 1.3224E-07 | < 3% | E | 2.0657E+07 | < 5% | D | 7.5617E+06 | < 5% | D |
| **METHYLALKENES** | | | | | | | | | | |
| 2-METHYL-2-BUTENE | 513-35-9 | - | - | - | 9.6127E+05 | < 3% | S | - | - | - |
| **N-ALCOHOLS** | | | | | | | | | | |
| METHANOL | 67-56-1 | - | - | - | 2.8376E+01 | < 5% | S | 1.6882E+00 | < 5% | S |
| ETHANOL | 64-17-5 | - | - | - | 3.1518E+01 | < 5% | S | 3.9792E+00 | < 5% | S |
| 1-PROPANOL | 71-23-8 | - | - | - | 3.9058E+01 | < 10% | S | 1.3915E+01 | < 10% | S |
| 1-BUTANOL | 71-36-3 | 1.8884E-02 | < 3% | S | 4.7161E+01 | < 5% | S | 5.2370E+01 | < 10% | S |
| 1-PENTANOL | 71-41-0 | 4.3266E-03 | < 3% | S | 6.3569E+01 | < 10% | S | 1.9216E+02 | < 10% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 1-HEXANOL | 111-27-3 | 1.0560E-03 | < 5% | S | 7.6111E+01 | < 25% | S | 7.7971E+02 | < 25% | S |
| 1-HEPTANOL | 111-70-6 | 2.4859E-04 | < 5% | S | 1.0435E+02 | < 10% | S | 3.5458E+03 | < 10% | S |
| 1-OCTANOL | 111-87-5 | 6.9824E-05 | < 10% | S | 1.5895E+02 | < 10% | S | 1.4289E+04 | < 10% | S |
| 1-NONANOL | 143-08-8 | 1.5673E-05 | < 25% | S | 2.0923E+02 | < 25% | S | 6.3464E+04 | < 25% | S |
| 1-DECANOL | 112-30-1 | 4.1701E-06 | < 10% | S | 3.0679E+02 | < 10% | S | 2.3876E+05 | < 10% | S |
| 1-UNDECANOL | 112-42-5 | 1.0330E-06 | < 50% | P | 4.0302E+02 | < 50% | P | 9.6801E+05 | < 50% | P |
| 1-DODECANOL | 112-53-8 | 2.5520E-07 | < 50% | P | 4.6684E+02 | < 50% | P | 3.9184E+06 | < 50% | P |
| 1-TRIDECANOL | 112-70-9 | 6.3040E-08 | < 50% | P | - | - | - | - | - | - |
| 1-TETRADECANOL | 112-72-1 | 1.5573E-08 | < 50% | P | - | - | - | - | - | - |
| 1-PENTADECANOL | 629-76-5 | 3.8469E-09 | < 100% | P | - | - | - | - | - | - |
| 1-HEXADECANOL | 36653-82-4 | 9.5034E-10 | < 100% | P | - | - | - | - | - | - |
| 1-HEPTADECANOL | 1454-85-9 | 2.3477E-10 | < 100% | P | - | - | - | - | - | - |
| 1-OCTADECANOL | 112-92-5 | 5.7993E-11 | < 100% | P | - | - | - | - | - | - |
| **N-ALIPHATIC PRIMARY AMINES** | | | | | | | | | | |
| METHYLAMINE | 74-89-5 | 1.0000E+00 | Unknown | E | - | - | - | - | - | - |
| ETHYLAMINE | 75-04-7 | 1.0000E+00 | Unknown | E | 6.6181E+01 | < 10% | S | 4.7374E-01 | < 25% | S |
| n-PROPYLAMINE | 107-10-8 | 1.0000E+00 | Unknown | E | 8.2550E+01 | < 10% | S | 1.9970E+00 | < 10% | S |
| n-BUTYLAMINE | 109-73-9 | 1.0000E+00 | Unknown | E | 1.0298E+02 | < 10% | S | 8.3162E+00 | < 10% | S |
| n-PENTYLAMINE | 110-58-7 | 1.0000E+00 | Unknown | E | 1.2844E+02 | < 10% | S | 3.2117E+01 | < 10% | S |
| n-HEXYLAMINE | 111-26-2 | - | - | - | 1.6021E+02 | < 10% | S | 1.3205E+02 | < 10% | S |
| n-HEPTYLAMINE | 111-68-2 | - | - | - | 1.9986E+02 | < 25% | S | 4.4889E+02 | < 25% | S |
| n-OCTYLAMINE | 111-86-4 | - | - | - | 2.4929E+02 | < 25% | S | 1.8558E+03 | < 25% | S |
| **N-ALKANES** | | | | | | | | | | |
| n-PENTANE | 109-66-0 | 1.0456E-05 | < 10% | S | 6.5485E+06 | < 10% | S | 9.5728E+04 | < 10% | S |
| n-HEXANE | 110-54-3 | 2.2390E-06 | < 10% | S | 9.0978E+06 | < 10% | S | 4.5143E+05 | < 10% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| n-HEPTANE | 142-82-5 | 4.7371E-07 | < 10% | S | 1.2916E+07 | < 10% | S | 2.1361E+06 | < 10% | S |
| n-OCTANE | 111-65-9 | 1.1329E-07 | < 25% | S | 1.6258E+07 | < 25% | S | 8.7203E+06 | < 25% | S |
| n-NONANE | 111-84-2 | 1.8576E-08 | < 50% | S | 3.0731E+07 | < 50% | S | 5.2941E+07 | < 50% | S |
| n-DECANE | 124-18-5 | 4.3460E-09 | < 50% | S | 4.1648E+07 | < 50% | S | 2.3009E+08 | < 50% | S |
| **N-ALKYLBENZENES** | | | | | | | | | | |
| BENZENE | 71-43-2 | 4.0652E-04 | < 3% | S | 3.1114E+04 | < 3% | S | 2.4561E+03 | < 3% | S |
| TOLUENE | 108-88-3 | 1.1535E-04 | < 3% | S | 3.3054E+04 | < 3% | S | 8.6874E+03 | < 5% | S |
| ETHYLBENZENE | 100-41-4 | 2.9892E-05 | < 3% | S | 4.2613E+04 | < 3% | S | 3.3370E+04 | < 5% | S |
| n-PROPYLBENZENE | 103-65-1 | 7.7818E-06 | < 10% | S | 5.9359E+04 | < 10% | S | 1.2796E+05 | < 10% | S |
| n-BUTYLBENZENE | 104-51-8 | 1.8154E-06 | < 5% | S | 7.8555E+04 | < 5% | S | 5.4877E+05 | < 5% | S |
| n-HEPTYLBENZENE | 1078-71-3 | 2.3098E-08 | < 5% | P | 2.0792E+05 | < 10% | P | 4.3293E+07 | < 5% | P |
| n-DECYLBENZENE | 104-72-3 | 2.0688E-10 | < 10% | S | 7.2846E+05 | < 10% | S | 4.8338E+09 | < 10% | S |
| n-PENTYLBENZENE | 538-68-1 | 4.3812E-07 | < 10% | S | 1.0026E+05 | < 10% | S | 2.2824E+06 | < 10% | S |
| n-HEXYLBENZENE | 1077-16-3 | 1.0832E-07 | < 3% | S | 1.3470E+05 | < 5% | S | 9.2359E+06 | < 10% | S |
| n-OCTYLBENZENE | 2189-60-8 | 4.9663E-09 | < 10% | P | 3.0050E+05 | < 10% | P | 2.0136E+08 | < 10% | P |
| n-NONYLBENZENE | 1081-77-2 | 1.0313E-09 | < 10% | P | 3.8660E+05 | < 25% | P | 9.6961E+08 | < 10% | P |
| **NAPHTHALENES** | | | | | | | | | | |
| NAPHTHALENE | 91-20-3 | 4.3668E-06 | < 3% | S | 2.5234E+03 | < 3% | S | 7.0849E+04 | < 5% | S |
| 1-METHYLNAPHTHALENE | 90-12-0 | 3.6833E-06 | < 10% | S | 2.7244E+03 | < 10% | S | 2.7144E+05 | < 10% | S |
| 2-METHYLNAPHTHALENE | 91-57-6 | 3.0163E-06 | < 25% | S | 2.7289E+03 | < 25% | S | 2.8517E+05 | < 25% | S |
| 1-ETHYLNAPHTHALENE | 1127-76-0 | 1.1956E-06 | < 10% | S | 2.7757E+03 | < 10% | S | 8.3651E+05 | < 10% | S |
| **NITRILES** | | | | | | | | | | |
| ACETONITRILE | 75-05-8 | - | - | - | 1.1210E+02 | < 5% | S | 9.2319E+00 | < 5% | S |
| PROPIONITRILE | 107-12-0 | 3.5087E-02 | < 10% | S | 1.6565E+02 | < 25% | S | 2.6265E+01 | < 25% | S |
| ACRYLONITRILE | 107-13-1 | 2.3502E-02 | < 3% | S | 5.4807E+02 | < 3% | S | 4.1682E+01 | < 25% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

|  |  | $x_i^{aq}$ (mol frac.) |  |  | $k_H$ (kPa) |  |  | $\gamma_i^{\infty}$ (unitless) |  |  |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| METHACRYLONITRILE | 126-98-7 | 5.9311E-03 | < 5% | S | 1.5916E+03 | < 5% | P | 1.6780E+02 | < 10% | P |
| SUCCINONITRILE | 110-61-2 | 2.2642E-02 | < 10% | S | - | - | - | - | - | - |
| GLUTARONITRILE | 544-13-8 | 1.9661E-02 | < 10% | S | - | - | - | - | - | - |
| n-BUTYRONITRILE | 109-74-0 | 8.8648E-03 | < 3% | S | 2.9080E+02 | < 3% | S | 1.1185E+02 | < 5% | S |
| VALERONITRILE | 110-59-8 | 2.7594E-03 | < 10% | S | 3.5359E+02 | < 25% | S | 3.6302E+02 | < 25% | S |
| ISOBUTYRONITRILE | 78-82-0 | 9.2527E-03 | < 5% | S | 5.0410E+02 | < 25% | S | 1.1538E+02 | < 25% | S |
| BENZONITRILE | 100-47-0 | 7.1412E-04 | < 25% | S | 1.6637E+02 | < 25% | S | 1.5605E+03 | < 25% | S |
| VINYLACETONITRILE | 109-75-1 | 8.8683E-03 | < 5% | S | 2.7177E+02 | < 1% | S | 1.1032E+02 | < 5% | S |
| PHENYLACETONITRILE | 140-29-4 | 2.6710E-04 | < 25% | S | 5.0250E+01 | < 100% | S | 4.0865E+03 | < 100% | S |
| **NITROAMINES** |  |  |  |  |  |  |  |  |  |  |
| o-NITROANILINE | 88-74-4 | 1.3507E-04 | < 50% | S | 7.7514E-01 | < 50% | S | 3.3338E+03 | < 100% | S |
| p-NITROANILINE | 100-01-6 | 7.4078E-05 | < 10% | S | 6.3686E-03 | < 10% | S | 1.6454E+03 | < 50% | S |
| m-NITROANILINE | 99-09-2 | 1.2221E-04 | < 10% | S | - | - | - | - | - | - |
| **ORGANIC SALTS** |  |  |  |  |  |  |  |  |  |  |
| DIETHYL CARBONATE | 105-58-8 | 2.6923E-03 | < 3% | S | 5.3166E+02 | < 3% | S | 3.6990E+02 | < 10% | S |
| DIMETHYL CARBONATE | 616-38-6 | 2.7871E-02 | < 3% | S | 3.5902E+02 | < 3% | S | 4.8661E+01 | < 5% | S |
| **OTHER ALIPHATIC ALCOHOLS** |  |  |  |  |  |  |  |  |  |  |
| ISOPROPANOL | 67-63-0 | - | - | - | 4.8094E+01 | < 10% | S | 8.2933E+00 | < 10% | S |
| 2-METHYL-1-PROPANOL | 78-83-1 | 2.1995E-02 | < 10% | S | 6.7391E+01 | < 10% | S | 4.8123E+01 | < 10% | S |
| 2-BUTANOL | 78-92-2 | 5.0591E-02 | < 3% | S | 5.9124E+01 | < 5% | S | 2.5291E+01 | < 5% | S |
| 2-METHYL-2-PROPANOL | 75-65-0 | - | - | - | 6.8926E+01 | < 5% | S | 1.2064E+01 | < 10% | S |
| 2-PENTANOL | 6032-29-7 | 8.8835E-03 | < 5% | S | 7.9763E+01 | < 3% | S | 9.8222E+01 | < 5% | S |
| 2-METHYL-2-BUTANOL | 75-85-4 | 2.4227E-02 | < 10% | S | 8.1409E+01 | < 3% | S | 3.5808E+01 | < 5% | S |
| 2-METHYL-1-BUTANOL | 137-32-6 | 5.4588E-03 | < 5% | S | 7.2382E+01 | < 5% | S | 1.4816E+02 | < 5% | S |
| 2,2-DIMETHYL-1-PROPANOL | 75-84-3 | 6.8035E-03 | < 10% | S | 1.7596E+02 | < 25% | P | 1.3088E+02 | < 25% | P |

## Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

|  |  | $x_i^{aq}$ (mol frac.) |  |  | $k_H$ (kPa) |  |  | $\gamma_i^{\infty}$ (unitless) |  |  |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 2-HEXANOL | 626-93-7 | 2.1193E-03 | < 5% | S | 1.4331E+02 | < 5% | S | 4.6989E+02 | < 10% | S |
| 3-HEXANOL | 623-37-0 | 2.7146E-03 | < 5% | S | 1.5227E+02 | < 3% | S | 3.6732E+02 | < 25% | S |
| 3-METHYL-1-PENTANOL | 589-35-5 | 1.6550E-03 | < 3% | S | 7.6763E+01 | < 10% | P | 5.9895E+02 | < 10% | P |
| 3-METHYL-3-PENTANOL | 77-74-7 | 6.1117E-03 | < 10% | S | 2.1990E+02 | < 10% | P | 1.6495E+02 | < 25% | P |
| 3-PENTANOL | 584-02-1 | 1.0665E-02 | < 3% | S | 9.2713E+01 | < 3% | S | 8.3949E+01 | < 5% | S |
| 3-METHYL-1-BUTANOL | 123-51-3 | 5.3033E-03 | < 5% | S | 6.9731E+01 | < 10% | S | 1.6643E+02 | < 25% | S |
| 3-METHYL-2-BUTANOL | 598-75-4 | 1.1849E-02 | < 5% | S | 1.1070E+02 | < 3% | S | 7.9081E+01 | < 10% | S |
| 2-HEPTANOL | 543-49-7 | 5.7725E-04 | < 5% | S | 1.7236E+02 | < 5% | P | 1.7183E+03 | < 10% | P |
| 3-HEPTANOL | 589-82-2 | 7.1191E-04 | < 10% | S | 1.7651E+02 | < 10% | S | 1.3947E+03 | < 10% | S |
| 4-METHYL-2-PENTANOL | 108-11-2 | 2.8026E-03 | < 10% | S | 2.4972E+02 | < 5% | S | 3.5580E+02 | < 10% | S |
| 2-OCTANOL | 123-96-6 | 1.5562E-04 | < 10% | S | 2.1047E+02 | < 10% | P | 6.3825E+03 | < 10% | P |
| 2-NONANOL | 628-99-9 | 3.8944E-05 | < 25% | S | 2.7628E+02 | < 25% | P | 2.5433E+04 | < 25% | P |
| 2,6-DIMETHYL-4-HEPTANOL | 108-82-7 | 7.5500E-05 | < 25% | S | 5.3226E+02 | < 25% | P | 1.3210E+04 | < 25% | P |
| **OTHER ALIPHATIC AMINES** |  |  |  |  |  |  |  |  |  |  |
| DIMETHYLAMINE | 124-40-3 | - | - | - | 8.9023E+01 | < 50% | S | - | - | - |
| TRIETHYLAMINE | 121-44-8 | 1.4394E-02 | < 10% | S | 5.9606E+02 | < 5% | S | 6.5469E+01 | < 5% | S |
| DI-n-PROPYLAMINE | 142-84-7 | 7.1637E-03 | < 25% | S | 2.5765E+02 | < 25% | S | 7.1297E+01 | < 25% | S |
| N,N-DIMETHYL-n-BUTYLAMINE | 927-62-8 | 4.7045E-03 | < 25% | S | - | - | - | - | - | - |
| N,N-DIETHYLMETHYLAMINE | 616-39-7 | 1.0000E+00 | Unknown | E | - | - | - | - | - | - |
| DIETHYLAMINE | 109-89-7 | 1.0000E+00 | Unknown | E | 1.5144E+02 | < 25% | S | 4.8211E+00 | < 25% | S |
| DIISOPROPYLAMINE | 108-18-9 | 1.0000E+00 | Unknown | E | - | - | - | - | - | - |
| DI-n-BUTYLAMINE | 111-92-2 | 6.8942E-04 | < 10% | S | 4.3834E+02 | < 50% | S | 1.2008E+03 | < 50% | S |
| TRI-n-BUTYLAMINE | 102-82-9 | 8.1648E-05 | < 25% | S | 1.4890E+02 | < 25% | S | 1.2208E+04 | < 25% | S |
| **OTHER ALKANES** |  |  |  |  |  |  |  |  |  |  |
| 2,3,4-TRIMETHYLPENTANE | 565-75-3 | 2.1260E-07 | < 5% | S | 1.7009E+07 | < 5% | S | 4.7045E+06 | < 5% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^\infty$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 2,2,5-TRIMETHYLHEXANE | 3522-94-9 | 7.5851E-08 | < 5% | E | 2.9316E+07 | < 10% | D | 1.3113E+07 | < 10% | D |
| **OTHER ALKYLBENZENES** | | | | | | | | | | |
| o-XYLENE | 95-47-6 | 3.2745E-05 | < 10% | S | 2.7047E+04 | < 10% | S | 3.0533E+04 | < 10% | S |
| m-XYLENE | 108-38-3 | 2.8685E-05 | < 5% | S | 3.8659E+04 | < 5% | S | 3.4498E+04 | < 10% | S |
| p-XYLENE | 106-42-3 | 2.9633E-05 | < 10% | S | 3.8088E+04 | < 10% | S | 3.2575E+04 | < 10% | S |
| CUMENE | 98-82-8 | 9.8434E-06 | < 5% | S | 6.1375E+04 | < 5% | S | 1.0110E+05 | < 10% | S |
| 1,2,3-TRIMETHYLBENZENE | 526-73-8 | 9.7333E-06 | < 25% | S | 2.3000E+04 | < 25% | S | 1.0645E+05 | < 25% | S |
| 1,2,4-TRIMETHYLBENZENE | 95-63-6 | 8.2984E-06 | < 5% | S | 3.4730E+04 | < 3% | S | 1.2134E+05 | < 5% | S |
| MESITYLENE | 108-67-8 | 7.4151E-06 | < 25% | S | 4.6913E+04 | < 25% | S | 1.3931E+05 | < 25% | S |
| p-DIETHYLBENZENE | 105-05-5 | 3.3790E-06 | < 100% | E | 2.8409E+04 | < 100% | D | 2.9628E+05 | < 100% | D |
| 1,2,3,4-TETRAMETHYLBENZENE | 488-23-3 | 2.3311E-06 | < 100% | S | 1.8900E+04 | < 100% | S | 4.2831E+05 | < 100% | S |
| 1,2,4,5-TETRAMETHYLBENZENE | 95-93-2 | 4.6710E-07 | < 10% | E | 4.0791E+04 | < 10% | D | 6.0549E+05 | < 25% | D |
| **OTHER AMINES, IMINES** | | | | | | | | | | |
| CYCLOHEXYLAMINE | 108-91-8 | 5.1435E-02 | Unknown | P | 2.4813E+01 | < 25% | S | 1.8486E+01 | < 25% | S |
| HEXAMETHYLENETETRAMINE | 100-97-0 | 9.3809E-02 | < 3% | S | - | - | - | - | - | - |
| N-ETHYL-2-METHYLALLYLAMINE | 18328-90-0 | 1.7908E-02 | < 25% | S | - | - | - | - | - | - |
| TRIALLYLAMINE | 102-70-5 | 3.5083E-04 | < 25% | S | 1.3674E+03 | < 10% | S | 2.8223E+03 | < 25% | S |
| N-METHYLCYCLOHEXYLAMINE | 100-60-7 | 6.4662E-03 | < 3% | S | - | - | - | - | - | - |
| DIALLYLAMINE | 124-02-7 | 2.0405E-02 | < 10% | S | - | - | - | - | - | - |
| N-METHYLPIPERIDINE | 626-67-5 | 1.0000E+00 | < 10% | E | - | - | - | - | - | - |
| **OTHER CONDENSED RINGS** | | | | | | | | | | |
| FLUORANTHENE | 206-44-0 | 2.1103E-08 | < 10% | S | 7.9065E+01 | < 10% | S | 1.0787E+07 | < 100% | S |
| FLUORENE | 86-73-7 | 1.9043E-07 | < 10% | S | 4.1834E+02 | < 10% | S | 1.1242E+06 | < 25% | S |
| ANTHRACENE | 120-12-7 | 4.6580E-09 | < 5% | S | 1.7268E+02 | < 5% | S | 4.3246E-01 | < 100% | S |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| PHENANTHRENE | 85-01-8 | 1.0729E-07 | < 5% | S | 1.6014E+02 | < 5% | S | 2.6089E+06 | < 10% | P |
| CHRYSENE | 218-01-9 | 1.3398E-10 | < 10% | S | 3.7646E+00 | < 10% | S | 2.1955E+08 | > 100% | P |
| PYRENE | 129-00-0 | 1.1600E-08 | < 5% | S | 4.9163E+01 | < 5% | S | 1.0798E+07 | < 10% | S |
| ACENAPHTHENE | 83-32-9 | 4.1124E-07 | < 25% | S | 7.7124E+02 | < 25% | S | 5.1573E+05 | < 25% | S |
| ACENAPHTHALENE | 208-96-8 | 1.5440E-06 | < 25% | S | 6.4945E+02 | < 25% | S | 3.9997E+05 | Unknown | S |
| BENZO[a]PYRENE | 50-32-8 | 1.1168E-10 | < 10% | S | 1.2412E+01 | < 5% | S | 1.6231E+09 | < 50% | S |
| BENZANTHRACENE | 56-55-3 | 7.0358E-10 | < 5% | S | - | - | - | - | - | - |
| BENZO[b]FLUORANTHENE | 205-99-2 | 1.0860E-10 | < 10% | S | 3.6764E+00 | < 10% | S | 2.7444E+08 | > 100% | S |
| **OTHER ETHERS/DIETHERS** | | | | | | | | | | |
| METHYLAL | 109-87-5 | 9.0588E-02 | < 5% | S | 9.0067E+02 | < 25% | S | 1.7117E+01 | < 25% | S |
| 1,2-DIMETHOXYETHANE | 110-71-4 | 6.7434E-02 | < 25% | S | 3.9438E+01 | < 3% | S | 4.2545E+00 | < 10% | S |
| DIETHYLENE GLYCOL DIETHYL ETHER | 112-36-7 | 1.0000E+00 | Unknown | E | - | - | - | - | - | - |
| DIETHYLENE GLYCOL DI-n-BUTYL ETHER | 112-73-2 | 1.6847E-04 | < 10% | S | 2.2058E+01 | > 100% | P | 6.2862E+03 | > 100% | P |
| ANISOLE | 100-66-3 | 2.4678E-04 | < 5% | S | 1.9271E+03 | < 5% | S | 4.0420E+03 | < 5% | S |
| DIPHENYL ETHER | 101-84-8 | 1.9486E-06 | < 5% | S | 2.9031E+03 | < 50% | S | 4.9071E+05 | < 50% | S |
| 1,2-DIETHOXYETHANE | 629-14-1 | 3.3244E-02 | < 5% | S | - | - | - | - | - | - |
| **OTHER INORGANICS** | | | | | | | | | | |
| HYDROGEN PEROXIDE | 7722-84-1 | - | - | - | 5.7967E-02 | < 25% | S | 2.2211E-01 | < 25% | S |
| **OTHER MONOAROMATICS** | | | | | | | | | | |
| STYRENE | 100-42-5 | 5.2493E-05 | < 5% | S | 1.5542E+04 | < 5% | S | 1.9043E+04 | < 5% | S |
| **OTHER POLYFUNCTIONAL C, H, O** | | | | | | | | | | |
| FURFURAL | 98-01-1 | 1.6437E-02 | < 5% | S | - | - | - | - | - | - |
| 2-BUTOXYETHANOL | 111-76-2 | 1.0000E+00 | < 3% | E | 4.3241E+00 | < 25% | S | 3.7889E+01 | < 25% | S |
| 2-HEXOXYETHANOL | 112-25-4 | 1.6257E-03 | < 25% | S | - | - | - | - | - | - |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| 2-(2-HEXOXYETHOXY)ETHANOL | 112-59-4 | 1.7793E-03 | < 25% | S | - | - | - | - | - | - |
| VANILLIN | 121-33-5 | 1.2265E-03 | < 3% | S | 3.1102E-02 | < 3% | S | 3.3360E+02 | < 50% | S |
| PROPYLENE GLYCOL n-BUTYL ETHER | 5131-66-8 | 7.7931E-03 | < 10% | S | - | - | - | - | - | - |
| **OTHER POLYFUNCTIONAL ORGANICS** | | | | | | | | | | |
| MALATHION | 121-75-5 | 8.4076E-06 | < 25% | S | 2.8250E+00 | < 3% | S | 1.1889E+05 | < 25% | S |
| THIOUREA | 62-56-6 | 3.7861E-02 | < 3% | S | - | - | - | - | - | - |
| **OTHER SATURATED ALIPHATIC ESTERS** | | | | | | | | | | |
| ETHYL ISOVALERATE | 108-64-5 | 2.7722E-04 | < 10% | S | 3.8440E+03 | < 10% | S | 3.5841E+03 | < 10% | S |
| DIETHYL MALONATE | 105-53-3 | 2.4991E-03 | < 5% | S | 1.4010E+01 | < 10% | P | 3.9755E+02 | < 25% | P |
| DIETHYL SUCCINATE | 123-25-1 | 2.1269E-03 | < 10% | S | - | - | - | - | - | - |
| ETHYL TRIMETHYL ACETATE | 3938-95-2 | 2.5561E-04 | < 25% | S | 8.7394E+03 | < 25% | S | 3.8894E+03 | < 25% | S |
| DIMETHYL SUCCINATE | 106-65-0 | 1.7223E-02 | < 3% | S | - | - | - | - | - | - |
| DIMETHYLMALONATE | 108-59-8 | 2.3027E-02 | < 10% | S | - | - | - | - | - | - |
| **PEROXIDES** | | | | | | | | | | |
| METHYL HYDROPEROXIDE | 3031-73-0 | - | - | - | 1.8200E+01 | < 5% | S | 3.7482E+00 | < 50% | S |
| ETHYL HYDROPEROXIDE | 3031-74-1 | - | - | - | 1.6528E+01 | < 10% | S | 4.5931E+00 | < 50% | S |
| **POLYFUNCTIONAL ACIDS** | | | | | | | | | | |
| SALICYLIC ACID | 69-72-7 | 2.8433E-04 | < 3% | S | - | - | - | - | - | - |
| **POLYFUNCTIONAL AMIDES/AMINES** | | | | | | | | | | |
| N,N-DIMETHYLFORMAMIDE | 68-12-2 | - | - | - | 3.6460E-01 | < 25% | S | 6.7237E-01 | < 50% | S |
| UREA | 57-13-6 | 2.5890E-01 | < 3% | S | - | - | - | - | - | - |
| N-METHYLFORMAMIDE | 123-39-7 | - | - | - | 4.0404E-02 | < 25% | S | 1.0955E+00 | < 25% | S |
| ACETAMIDE | 60-35-5 | 4.3874E-01 | < 1% | S | - | - | - | - | - | - |
| N,N-DIMETHYLACETAMIDE | 127-19-5 | - | - | - | 1.2519E-01 | < 50% | P | 4.3060E-01 | < 50% | P |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| N,N-DIETHYLHYDROXYLAMINE | 3710-84-7 | 1.0021E-01 | < 3% | S | - | - | - | - | - | - |
| **POLYFUNCTIONAL C, H, N, HALIDE, (O)** | | | | | | | | | | |
| o-CHLOROANILINE | 95-51-2 | 1.2271E-03 | < 25% | S | 2.6749E+01 | < 25% | P | 8.0958E+02 | < 25% | P |
| p-CHLORONITROBENZENE | 100-00-5 | 2.8118E-05 | < 10% | S | 8.6341E+01 | < 10% | S | 2.1744E+04 | < 50% | S |
| **POLYFUNCTIONAL C, H, O, HALIDE** | | | | | | | | | | |
| DI(2-CHLOROETHYL)ETHER | 111-44-4 | 1.2915E-03 | < 3% | S | 1.1134E+02 | < 3% | S | 7.7156E+02 | < 10% | S |
| ETHYLCHLOROACETATE | 105-39-5 | 2.9808E-03 | < 5% | S | 2.1209E+02 | < 10% | S | 3.3591E+02 | < 25% | S |
| o-CHLOROPHENOL | 95-57-8 | 3.2052E-03 | < 3% | S | - | - | - | - | - | - |
| m-CHLOROPHENOL | 108-43-0 | 3.2188E-03 | < 5% | S | - | - | - | - | - | - |
| p-CHLOROPHENOL | 106-48-9 | 3.3222E-03 | < 25% | S | - | - | - | - | - | - |
| METHYL CHLOROACETATE | 96-34-4 | 8.8232E-03 | < 3% | S | 1.1352E+02 | < 3% | S | 1.1243E+02 | < 5% | S |
| **POLYFUNCTIONAL C, H, O, N** | | | | | | | | | | |
| N-METHYL-2-PYRROLIDONE | 872-50-4 | - | - | - | 1.6824E-02 | < 10% | S | 3.6610E-01 | < 10% | S |
| ACETAMINOPHEN | 103-90-2 | 1.7020E-03 | < 3% | S | - | - | - | - | - | - |
| ACETANILIDE | 103-84-4 | 8.1951E-04 | < 10% | S | - | - | - | - | - | - |
| **POLYFUNCTIONAL C, H, O, S** | | | | | | | | | | |
| DIMETHYL SULFOXIDE | 67-68-5 | - | - | - | 6.9311E-03 | < 25% | S | 8.5921E-02 | < 25% | S |
| **POLYFUNCTIONAL ESTERS** | | | | | | | | | | |
| METHYL SALICYLATE | 119-36-8 | 1.5371E-04 | < 10% | S | 3.3064E+01 | < 25% | S | 6.4658E+03 | < 25% | S |
| 2-ETHOXYETHYL ACETATE | 111-15-9 | 3.8954E-02 | < 5% | S | 1.8500E+01 | < 10% | E | | | |
| ETHYL ACETOACETATE | 141-97-9 | 1.5712E-02 | < 25% | S | 6.1986E+00 | < 25% | S | 6.5389E+01 | < 25% | S |
| ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE | 112-07-2 | 1.7864E-03 | < 25% | S | 3.0618E+01 | < 25% | E | 2.6500E+02 | < 25% | D |
| **POLYOLS** | | | | | | | | | | |
| p-HYDROQUINONE | 123-31-9 | 1.2199E-02 | < 3% | S | - | - | - | - | - | - |

## Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| XYLITOL | 87-99-0 | 1.7785E-01 | < 5% | S | - | - | - | - | - | - |
| 1,3-BENZENEDIOL | 108-46-3 | 2.1628E-01 | < 3% | S | - | - | - | - | - | - |
| **PROPIONATES AND BUTYRATES** | | | | | | | | | | |
| METHYL PROPIONATE | 554-12-1 | 1.2818E-02 | < 3% | S | 9.6262E+02 | < 5% | S | 8.4969E+01 | < 5% | S |
| ETHYL PROPIONATE | 105-37-3 | 3.4032E-03 | < 25% | S | 1.4323E+03 | < 25% | S | 2.9291E+02 | < 25% | S |
| n-PROPYL PROPIONATE | 106-36-5 | 9.0986E-04 | < 10% | S | 2.0359E+03 | < 10% | S | 1.0930E+03 | < 10% | S |
| n-BUTYL PROPIONATE | 590-01-2 | 2.4314E-04 | < 5% | S | 2.4355E+03 | < 5% | S | 4.0803E+03 | < 10% | S |
| n-PROPYL n-BUTYRATE | 105-66-8 | 2.5274E-04 | < 25% | S | 3.0510E+03 | < 25% | S | 3.9278E+03 | < 25% | S |
| METHYL n-BUTYRATE | 623-42-7 | 3.0473E-03 | < 25% | S | 1.3329E+03 | < 25% | S | 3.1059E+02 | < 25% | E |
| ETHYL n-BUTYRATE | 105-54-4 | 1.0223E-03 | < 10% | S | 2.1767E+03 | < 10% | S | 9.7580E+02 | < 10% | S |
| ISOBUTYL ISOBUTYRATE | 97-85-8 | 7.3381E-05 | < 25% | S | 7.9493E+03 | < 25% | S | 1.3565E+04 | < 25% | S |
| n-BUTYL n-BUTYRATE | 109-21-7 | 7.9584E-05 | < 10% | S | 3.4019E+03 | < 10% | S | 1.2443E+04 | < 10% | S |
| METHYL ISOBUTYRATE | 547-63-7 | 3.1917E-03 | < 3% | S | 2.0910E+03 | < 10% | S | 3.1234E+02 | < 10% | S |
| ETHYL ISOBUTYRATE | 97-62-1 | 9.5920E-04 | < 10% | S | 3.5044E+03 | < 10% | P | 1.0373E+03 | < 10% | P |
| n-PENTYL n-BUTYRATE | 540-18-1 | 3.1389E-05 | < 25% | S | 3.3166E+03 | < 25% | S | 3.1692E+04 | < 25% | S |
| ISOPENTYL BUTYRATE | 106-27-4 | 2.7546E-05 | < 100% | S | 5.2634E+03 | < 100% | S | 3.6102E+04 | < 100% | S |
| **SULFIDES/THIOPHENES** | | | | | | | | | | |
| DIMETHYL SULFIDE | 75-18-3 | 6.1242E-03 | < 10% | S | 1.0548E+04 | < 10% | S | 1.6343E+02 | < 10% | S |
| DIMETHYL DISULFIDE | 624-92-0 | 5.6992E-04 | < 10% | P | 6.6448E+03 | < 10% | S | 1.7561E+03 | < 10% | S |
| 2-METHYLTHIOPHENE | 554-14-3 | 2.4374E-04 | < 10% | S | 1.3663E+04 | < 10% | S | 4.0928E+03 | < 10% | S |
| DIISOPROPYL SULFIDE | 625-80-9 | 1.3264E-04 | < 25% | S | 1.9586E+04 | < 10% | S | 7.4705E+03 | < 25% | S |
| **UNSATURATED ALIPHATIC ESTERS** | | | | | | | | | | |
| ETHYL ACRYLATE | 140-88-5 | 3.5978E-03 | < 10% | S | 1.4139E+03 | < 10% | P | 2.7901E+02 | < 10% | P |
| METHYL METHACRYLATE | 80-62-6 | 2.7645E-03 | < 3% | S | 1.8891E+03 | < 3% | S | 3.8100E+02 | < 10% | S |
| DIETHYL MALEATE | 141-05-9 | 1.5787E-03 | < 3% | S | - | - | - | - | - | - |

Table C.5: Summary of constant value recommendations (298.15 K and 1 atm) (cont.)

| | | $x_i^{aq}$ (mol frac.) | | | $k_H$ (kPa) | | | $\gamma_i^{\infty}$ (unitless) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Name | CAS | Value | s | DT | Value | s | DT | Value | s | DT |
| DIMETHYL MALEATE | 624-48-6 | 1.0309E-02 | < 3% | S | - | - | - | - | - | - |

# Appendix D. Experimental Data

Details of each experimental run are included in this appendix. The abbreviations of the headings are given in Table D.1. Any variables not included in the table are described in Section 5.2.

Table D.1: Abbreviations used in tables with experimental run information

| | |
|---|---|
| ID | Experimental run number |
| ChemID | 502 = toluene, 1105 = 1-butanol, 1461 = anisole, 1637 = 1,2-difluorobenzene, 2592 = 1,2,3-trichlorobenzene, 2661 = 4-bromotoluene, 1579 = 2,4-dichlorotoluene |
| Date | Date of experiment |
| Cell Order | Experimental number with a given cell |
| Cell T | Cell temperature |
| Room T | Room temperature |
| Cell P | Cell pressure |
| Flow Rate | $N_2$ flow rate at room temperature |
| n | Number of GC measurements used to calculate the slope, $a$ |
| $a$ | Slope (Equation 5.23) |
| $s_k$ | Error of variable $k$ |
| $R^2$ | $R^2$ of plot used to obtain $a$ |
| $H_2O$ (g) | Water in stripping cell |
| Solute | Initial amount of solute; values only included for the first cell run |
| $y_i$ max | The maximum headspace concentration possible due to the initial amount of solute |
| use | Y = run was included when determining final value; N = adsorption effects were significant so run was not included |

Table D.2: Cell data for each experimental run

| ID | ChemID | Date | Cell Order | Cell T (K) | Room T (K) | Cell P (atm) | $H_2O$ (g) | Solute | $y_i$ max |
|---|---|---|---|---|---|---|---|---|---|
| 116 | 502 | 1/4/2012 | 1 | 298.15 | 296.99 | 0.887 | 356.518 | 0.156 g | 3.09E-02 |
| 133 | 502 | 3/29/2012 | 8 | 298.15 | 296.99 | 0.859 | 394.566 | | |
| 135 | 502 | 3/30/2012 | 2 | 298.15 | 296.99 | 0.872 | 395.055 | | |
| 123 | 502 | 3/21/2012 | 2 | 298.15 | 296.99 | 0.852 | 393.915 | | |
| 126 | 502 | 3/23/2012 | 2 | 298.15 | 296.99 | 0.870 | 394.566 | | |
| 117 | 502 | 1/4/2012 | 2 | 298.15 | 296.99 | 0.871 | 356.518 | | |
| 116 | 502 | 12/15/2012 | 1 | 298.15 | 296.99 | 0.904 | 352.976 | 0.03 g | |
| 118 | 502 | 1/20/2012 | 1 | 298.15 | 296.99 | 0.851 | 362.157 | 0.112 g | 2.07E-02 |
| 119 | 502 | 1/20/2012 | 2 | 298.15 | 296.99 | 0.872 | 362.157 | | |
| 122 | 502 | 3/21/2012 | 1 | 298.15 | 296.99 | 0.906 | 393.915 | 0.12 mL | 2.07E-02 |
| 124 | 502 | 3/22/2012 | 3 | 298.15 | 296.99 | 0.901 | 393.915 | | |
| 125 | 502 | 3/23/2012 | 1 | 298.15 | 296.99 | 0.901 | 394.566 | 0.133 g | 1.89E-02 |
| 128 | 502 | 3/26/2012 | 3 | 298.15 | 296.99 | 0.845 | 394.566 | | |
| 129 | 502 | 3/26/2012 | 4 | 298.15 | 296.99 | 0.900 | 394.566 | | |
| 130 | 502 | 3/26/2012 | 5 | 298.15 | 296.99 | 0.872 | 394.566 | | |
| 131 | 502 | 3/29/2012 | 6 | 298.15 | 296.99 | 0.909 | 394.566 | | |
| 132 | 502 | 3/29/2012 | 7 | 298.15 | 296.99 | 0.866 | 394.566 | | |
| 134 | 502 | 3/30/2012 | 1 | 298.15 | 296.99 | 0.859 | 395.055 | | |
| 120 | 502 | 1/30/2012 | 1 | 308.15 | 296.99 | 0.850 | 387.738 | 0.125 g | 3.27E-02 |
| 121 | 502 | 1/30/2012 | 2 | 308.15 | 296.99 | 0.871 | 387.738 | | |
| 5 | 1105 | 4/11/2012 | 4 | 298.15 | 296.99 | 1.031 | 375.291 | | |
| 2 | 1105 | 4/10/2012 | 1 | 308.15 | 296.99 | 1.043 | 375.291 | 4.265 g | 2.86E-03 |
| 4 | 1105 | 4/11/2012 | 3 | 313.15 | 296.99 | 1.042 | 375.291 | | |
| 1 | 1105 | 4/6/2012 | 1 | 323.15 | 297.02 | 1.063 | 396.165 | 0.9246 g | 1.56E-03 |
| 3 | 1105 | 4/10/2012 | 2 | 323.15 | 296.99 | 1.058 | 375.291 | | |
| 103 | 1461 | 5/30/2012 | 1 | 281.05 | 296.85 | 1.046 | 388.706 | 0.42 g | 1.37E-03 |
| 107 | 1461 | 5/30/2012 | 5 | 281.06 | 296.35 | 1.039 | 388.706 | | |
| 92 | 1461 | 5/25/2012 | 3 | 293.12 | 297.05 | 1.027 | 390.332 | | |
| 89 | 1461 | 5/24/2012 | 3 | 293.14 | 298.35 | 1.034 | 394.685 | | |
| 88 | 1461 | 5/24/2012 | 2 | 293.18 | 298.75 | 1.036 | 394.685 | | |
| 101 | 1461 | 5/29/2012 | 6 | 281.04 | 296.65 | 1.037 | 389.472 | | |
| 102 | 1461 | 5/29/2012 | 7 | 281.04 | 296.65 | 1.031 | 389.472 | | |
| 108 | 1461 | 5/31/2012 | 6 | 281.04 | 296.95 | 1.044 | 388.706 | | |
| 100 | 1461 | 5/29/2012 | 5 | 281.05 | 297.25 | 1.040 | 389.472 | | |
| 111 | 1461 | 6/1/2012 | 2 | 281.07 | 296.45 | 1.045 | 390.316 | | |
| 113 | 1461 | 6/6/2012 | 2 | 281.07 | 298.15 | 1.036 | 387.785 | | |
| 115 | 1461 | 6/7/2012 | 4 | 281.07 | 298.45 | 1.039 | 387.785 | | |

Table D.2: Cell data for each experimental run (cont.)

| ID | ChemID | Date | Cell Order | Cell T (K) | Room T (K) | Cell P (atm) | $H_2O$ (g) | Solute | $y_i$ max |
|---|---|---|---|---|---|---|---|---|---|
| 109 | 1461 | 5/31/2012 | 7 | 281.09 | 296.75 | 1.041 | 388.706 | | |
| 90 | 1461 | 5/25/2012 | 1 | 293.1 | 297.55 | 0.940 | 390.332 | 0.458 g | 2.74E-03 |
| 106 | 1461 | 5/30/2012 | 4 | 293.12 | 296.35 | 0.996 | 388.706 | | |
| 93 | 1461 | 5/26/2012 | 4 | 293.16 | 297.75 | 0.986 | 390.332 | | |
| 91 | 1461 | 5/25/2012 | 2 | 293.18 | 297.05 | 0.978 | 390.332 | | |
| 112 | 1461 | 6/6/2012 | 1 | 293.19 | 298.45 | 0.998 | 387.785 | 0.343 g | 2.15E-03 |
| 114 | 1461 | 6/7/2012 | 3 | 293.2 | 298.65 | 0.995 | 387.785 | | |
| 99 | 1461 | 5/28/2012 | 4 | 308.11 | 296.75 | 0.998 | 389.472 | | |
| 105 | 1461 | 5/30/2012 | 3 | 308.14 | 296.25 | 1.001 | 388.706 | | |
| 97 | 1461 | 5/28/2012 | 2 | 308.17 | 296.95 | 0.975 | 389.472 | | |
| 104 | 1461 | 5/30/2012 | 2 | 308.19 | 296.35 | 1.001 | 388.706 | | |
| 96 | 1461 | 5/28/2012 | 1 | 322.87 | 296.65 | 0.975 | 389.472 | 0.46 g | 1.06E-02 |
| 98 | 1461 | 5/28/2012 | 3 | 322.9 | 296.65 | 0.971 | 389.472 | | |
| 94 | 1461 | 5/26/2012 | 5 | 322.91 | 297.25 | 1.007 | 390.332 | | |
| 110 | 1461 | 6/1/2012 | 1 | 322.91 | 296.65 | 1.017 | 390.316 | 0.43 g | 1.00E-02 |
| 95 | 1461 | 5/26/2012 | 6 | 322.92 | 297.75 | 0.965 | 390.332 | | |
| 35 | 1637 | 4/13/2012 | 4 | 298.15 | 296.99 | 0.901 | 394.062 | | |
| 40 | 1637 | 4/16/2012 | 5 | 298.15 | 296.99 | 0.911 | 394.542 | | |
| 38 | 1637 | 4/16/2012 | 3 | 298.15 | 296.99 | 0.855 | 394.542 | | |
| 39 | 1637 | 4/16/2012 | 4 | 298.15 | 296.99 | 0.895 | 394.542 | | |
| 59 | 1637 | 5/2/2012 | 3 | 298.15 | 297.15 | 0.885 | 394.516 | | |
| 57 | 1637 | 5/2/2012 | 1 | 298.15 | 297.15 | 0.905 | 394.516 | 0.25 g | 3.43E-02 |
| 61 | 1637 | 5/3/2012 | 5 | 298.18 | 296.85 | 0.904 | 394.516 | | |
| 62 | 1637 | 5/3/2012 | 6 | 298.18 | 296.65 | 0.886 | 394.516 | | |
| 33 | 1637 | 4/13/2012 | 2 | 298.35 | 296.99 | 0.844 | 394.062 | | |
| 41 | 1637 | 4/17/2012 | 1 | 298.35 | 296.99 | 0.855 | 392.354 | 0.201 g | 2.46E-02 |
| 34 | 1637 | 4/13/2012 | 3 | 298.35 | 296.99 | 0.884 | 394.062 | | |
| 36 | 1637 | 4/16/2012 | 1 | 298.35 | 296.99 | 0.913 | 394.542 | 0.21 g | 3.25E-02 |
| 50 | 1637 | 4/24/2012 | 3 | 308.15 | 295.95 | 0.874 | 396.527 | | |
| 47 | 1637 | 4/23/2012 | 2 | 317.9 | 296.95 | 0.879 | 394.874 | | |
| 44 | 1637 | 4/17/2012 | 4 | 323.15 | 296.99 | 0.882 | 392.354 | | |
| 45 | 1637 | 4/17/2012 | 5 | 323.15 | 296.99 | 0.883 | 392.354 | | |
| 58 | 1637 | 5/2/2012 | 2 | 298.13 | 297.15 | 0.854 | 394.516 | | |
| 60 | 1637 | 5/3/2012 | 4 | 298.14 | 296.95 | 0.854 | 394.516 | | |
| 37 | 1637 | 4/16/2012 | 2 | 298.15 | 296.99 | 0.880 | 394.542 | | |
| 32 | 1637 | 4/13/2012 | 1 | 298.35 | 296.99 | 0.871 | 394.062 | 0.198 g | 3.44E-02 |
| 51 | 1637 | 4/26/2012 | 1 | 308.05 | 296.85 | 0.870 | 396.177 | 0.264 g | 7.17E-02 |

Table D.2: Cell data for each experimental run (cont.)

| ID | ChemID | Date | Cell Order | Cell T (K) | Room T (K) | Cell P (atm) | $H_2O$ (g) | Solute | $y_i$ max |
|---|---|---|---|---|---|---|---|---|---|
| 42 | 1637 | 4/17/2012 | 2 | 308.15 | 296.99 | 0.881 | 392.354 | | |
| 43 | 1637 | 4/17/2012 | 3 | 308.15 | 296.99 | 0.881 | 392.354 | | |
| 52 | 1637 | 4/26/2012 | 2 | 317.89 | 296.65 | 0.870 | 396.177 | | |
| 48 | 1637 | 4/24/2012 | 1 | 317.9 | 296.15 | 0.878 | 396.527 | 0.243 g | 9.01E-02 |
| 53 | 1637 | 4/27/2012 | 1 | 317.92 | 297.65 | 0.881 | 393.315 | 0.24 g | 8.60E-02 |
| 54 | 1637 | 4/27/2012 | 2 | 322.79 | 297.75 | 0.881 | 393.315 | | 2.12E-03 |
| 55 | 1637 | 4/27/2012 | 1 | 322.82 | 297.65 | 0.881 | 393.308 | 0.25 g | 1.08E-01 |
| 56 | 1637 | 4/27/2012 | 2 | 322.83 | 298.15 | 0.880 | 393.308 | | 3.50E-03 |
| 46 | 1637 | 4/23/2012 | 1 | 322.95 | 296.15 | 0.882 | 394.874 | 0.186 g | 8.10E-02 |
| 49 | 1637 | 4/24/2012 | 2 | 323.05 | 295.65 | 0.878 | 396.527 | | |
| 62.5 | 2592 | 5/14/2012 | | 293.1 | 297.15 | 0.881 | 394.228 | 0.002 g | |
| 82 | 2592 | 6/4/2012 | 1 | 281.04 | 296.45 | 0.891 | 394.028 | | |
| 83 | 2592 | 6/4/2012 | 2 | 281.06 | 296.45 | 0.907 | 394.028 | | |
| 84 | 2592 | 6/4/2012 | 3 | 281.07 | 297.05 | 0.904 | 394.028 | | |
| 86 | 2592 | 6/5/2012 | 5 | 281.07 | 297.15 | 0.902 | 394.028 | | |
| 85 | 2592 | 6/5/2012 | 4 | 281.08 | 296.25 | 0.899 | 394.028 | | |
| 68 | 2592 | 5/16/2012 | 6 | 292.8 | 296.35 | 0.948 | 395.873 | | |
| 67 | 2592 | 5/16/2012 | 5 | 292.95 | 296.25 | 0.873 | 395.873 | | |
| 65 | 2592 | 5/15/2012 | 3 | 293.1 | 296.65 | 0.911 | 395.873 | | |
| 66 | 2592 | 5/15/2012 | 4 | 293.11 | 297.35 | 0.948 | 395.873 | | |
| 69 | 2592 | 5/16/2012 | 7 | 293.11 | 296.15 | 0.907 | 395.873 | | |
| 70 | 2592 | 5/16/2012 | 8 | 293.11 | 296.25 | 0.889 | 395.873 | | |
| 63 | 2592 | 5/15/2012 | 1 | 293.15 | 297.15 | 0.894 | 395.873 | 0.002 g | 2.85E-05 |
| 79 | 2592 | 5/23/2012 | 4 | 293.21 | 297.65 | 0.888 | 392.05 | | |
| 71 | 2592 | 5/16/2012 | 1 | 308.1 | 296.99 | 0.891 | 395.47 | 0.002 g | 7.31E-05 |
| 72 | 2592 | 5/17/2012 | 2 | 308.1 | 296.99 | 0.837 | 395.47 | | |
| 73 | 2592 | 5/17/2012 | 3 | 308.1 | 296.99 | 0.837 | 395.47 | | |
| 81 | 2592 | 5/23/2012 | 6 | 308.18 | 297.15 | 0.887 | 392.05 | | |
| 80 | 2592 | 5/23/2012 | 5 | 308.22 | 297.35 | 0.889 | 392.05 | | |
| 74 | 2592 | 5/18/2012 | 4 | 322.85 | 296.99 | 0.898 | 395.47 | | |
| 75 | 2592 | 5/18/2012 | 5 | 322.87 | 296.99 | 0.898 | 395.47 | | |
| 76 | 2592 | 5/22/2012 | 1 | 322.97 | 296.35 | 0.896 | 392.05 | 0.002 g | 1.46E-04 |
| 77 | 2592 | 5/22/2012 | 2 | 322.97 | 296.35 | 0.896 | 392.05 | | |
| 78 | 2592 | 5/22/2012 | 3 | 322.97 | 296.05 | 0.896 | 392.05 | | |
| 31 | 2661 | 5/12/2012 | 5 | 293.12 | 298.15 | 0.881 | 395.451 | | |
| 10 | 2661 | 5/8/2012 | 1 | 308.07 | 297.15 | 0.864 | 394.770 | 0.020 g | 1.04E-03 |
| 20 | 2661 | 5/11/2012 | 3 | 322.9 | 297.25 | 0.880 | 395.451 | | |

Table D.2: Cell data for each experimental run (cont.)

| ID | ChemID | Date | Cell Order | Cell T (K) | Room T (K) | Cell P (atm) | $H_2O$ (g) | Solute | $y_i$ max |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 2661 | 5/10/2012 | 5 | 293.07 | 297.25 | 0.872 | 394.844 | | |
| 27 | 2661 | 5/10/2012 | 6 | 293.09 | 297.15 | 0.872 | 394.844 | | |
| 30 | 2661 | 5/11/2012 | 1 | 293.15 | 297.45 | 0.876 | 395.451 | 0.020 g | 6.10E-04 |
| 29 | 2661 | 5/10/2012 | 9 | 298.13 | 296.95 | 0.872 | 394.844 | | |
| 28 | 2661 | 5/10/2012 | 7 | 298.14 | 297.05 | 0.873 | 394.844 | | |
| 25 | 2661 | 5/4/2012 | 1 | 298.2 | 297.85 | 0.874 | 393.956 | 0.0005 g | 2.41E-05 |
| 12 | 2661 | 5/8/2012 | 3 | 308.05 | 297.15 | 0.897 | 394.770 | | |
| 17 | 2661 | 5/9/2012 | 4 | 308.07 | 295.65 | 0.892 | 394.844 | | |
| 16 | 2661 | 5/9/2012 | 3 | 308.08 | 295.65 | 0.911 | 394.844 | | |
| 8 | 2661 | 5/7/2012 | 4 | 308.093 | 297.35 | 0.876 | 393.956 | | |
| 6 | 2661 | 5/7/2012 | 2 | 308.1 | 297.65 | 0.895 | 393.956 | 0.030 g | 2.18E-03 |
| 9 | 2661 | 5/7/2012 | 5 | 308.1 | 295.65 | 0.912 | 393.956 | | |
| 13 | 2661 | 5/8/2012 | 4 | 308.1 | 296.65 | 0.878 | 394.770 | | |
| 15 | 2661 | 5/9/2012 | 2 | 308.1 | 296.95 | 0.877 | 394.844 | | |
| 21 | 2661 | 5/11/2012 | 4 | 308.1 | 297.35 | 0.876 | 395.451 | | |
| 7 | 2661 | 5/7/2012 | 3 | 308.15 | 297.65 | 0.861 | 393.956 | | |
| 11 | 2661 | 5/8/2012 | 2 | 308.15 | 297.25 | 0.916 | 394.770 | | |
| 14 | 2661 | 5/9/2012 | 1 | 308.15 | 297.25 | 0.862 | 394.844 | 0.020 g | 1.47E-03 |
| 24 | 2661 | 5/12/2012 | 8 | 317.95 | 296.75 | 0.881 | 395.451 | | |
| 18 | 2661 | 5/10/2012 | 8 | 318.1 | 295.75 | 0.875 | 394.844 | | |
| 22 | 2661 | 5/12/2012 | 6 | 322.89 | 297.05 | 0.885 | 395.451 | | |
| 19 | 2661 | 5/11/2012 | 2 | 322.91 | 297.65 | 0.881 | 395.451 | | |
| 23 | 2661 | 5/12/2012 | 7 | 322.92 | 297.05 | 0.884 | 395.451 | | |
| 136 | 1461 | 8/28/2012 | 1 | 280.96 | 296.35 | 0.992 | 386.149 | 0.420 g | |
| 137 | 1461 | 8/28/2012 | 2 | 280.97 | 297.15 | 0.990 | 386.149 | | |
| 138 | 1461 | 8/28/2012 | 3 | 280.95 | 297.15 | 0.988 | 386.149 | | |
| 139 | 1461 | 8/28/2012 | 4 | 280.94 | 297.35 | 0.987 | 386.149 | | |
| 140 | 1461 | 8/29/2012 | 5 | 280.95 | 296.85 | 0.992 | 386.149 | | |
| 141 | 2592 | 8/30/2012 | 1 | 293.1 | 297.35 | 0.878 | 394.989 | 0.002 g | |
| 142 | 2592 | 8/30/2012 | 2 | 293.09 | 297.15 | 0.862 | 394.989 | | |
| 143 | 2592 | 8/30/2012 | 3 | 323.08 | 297.15 | 0.882 | 394.989 | | |
| 144 | 2592 | 8/30/2012 | 4 | 323.14 | 296.95 | 0.880 | 394.989 | | |
| 145 | 2592 | 8/31/2012 | 5 | 323.09 | 296.95 | 0.886 | 394.989 | | |
| 146 | 2592 | 8/31/2012 | 6 | 308.12 | 296.95 | 0.879 | 394.989 | | |
| 147 | 2592 | 8/31/2012 | 7 | 280.95 | 297.05 | 0.876 | 394.989 | | |
| 148 | 2592 | 9/3/2012 | 1 | 293.09 | 296.95 | 0.881 | 393.47 | 0.002 g | |
| 149 | 2592 | 9/3/2012 | 2 | 280.94 | 297.15 | 0.862 | 393.47 | | |

Table D.2: Cell data for each experimental run (cont.)

| ID | ChemID | Date | Cell Order | Cell T (K) | Room T (K) | Cell P (atm) | $H_2O$ (g) | Solute | $y_i$ max |
|---|---|---|---|---|---|---|---|---|---|
| 150 | 2592 | 9/3/2012 | 3 | 280.95 | 297.25 | 0.860 | 393.47 | | |
| 151 | 2592 | 9/3/2012 | 4 | 280.96 | 297.25 | 0.862 | 393.47 | | |
| 177 | 1579 | 9/24/2012 | 2 | 323.09 | 297.25 | 0.886 | 395.214 | 0.013 g | 5.38E-03 |
| 165 | 1579 | 9/10/2012 | 5 | 280.91 | 297.05 | 0.896 | 395.521 | | |
| 176 | 1579 | 9/24/2012 | 1 | 280.95 | 297.45 | 0.896 | 395.214 | 0.0077 g | 1.72E-04 |
| 178 | 1579 | 9/24/2012 | 4 | 280.93 | 298.05 | 0.892 | 395.214 | | |
| 174 | 1579 | 9/14/2012 | 3 | 280.96 | 297.95 | 0.900 | 394.095 | | |
| 158 | 1579 | 9/6/2012 | 7 | 293.09 | 297.25 | 0.861 | 395.495 | | |
| 154 | 1579 | 9/5/2012 | 3 | 293.1 | 297.15 | 0.864 | 395.495 | | |
| 163 | 1579 | 9/7/2012 | 3 | 293.11 | 297.55 | 0.867 | 395.521 | | |
| 160 | 1579 | 9/6/2012 | 9 | 293.07 | 297.15 | 0.876 | 395.495 | | |
| 157 | 1579 | 9/6/2012 | 6 | 293.09 | 297.15 | 0.877 | 395.495 | | |
| 159 | 1579 | 9/6/2012 | 8 | 293.09 | 297.15 | 0.877 | 395.495 | | |
| 161 | 1579 | 9/7/2012 | 1 | 293.11 | 297.25 | 0.884 | 395.521 | 0.0092 g | 4.08E-04 |
| 173 | 1579 | 9/14/2012 | 2 | 293.07 | 298.55 | 0.903 | 394.095 | | |
| 155 | 1579 | 9/5/2012 | 4 | 293.08 | 297.05 | 0.896 | 395.495 | | |
| 153 | 1579 | 9/5/2012 | 2 | 293.09 | 297.25 | 0.898 | 395.495 | | |
| 162 | 1579 | 9/7/2012 | 2 | 293.09 | 297.65 | 0.901 | 395.521 | | |
| 156 | 1579 | 9/6/2012 | 5 | 293.07 | 296.95 | 0.912 | 395.495 | | |
| 152 | 1579 | 9/5/2012 | 1 | 293.1 | 297.25 | 0.916 | 395.495 | 0.0092 g | 4.95E-04 |
| 164 | 1579 | 9/7/2012 | 4 | 293.12 | 297.25 | 0.917 | 395.521 | | |
| 172 | 1579 | 9/14/2012 | 1 | 308.14 | 298.15 | 0.888 | 394.095 | 0.01 g | 9.04E-04 |
| 168 | 1579 | 9/11/2012 | 1 | 308.15 | 297.05 | 0.898 | 395.133 | | |
| 169 | 1579 | 9/11/2012 | 2 | 308.15 | 297.05 | 0.897 | 395.133 | | |
| 166 | 1579 | 9/10/2012 | 6 | 308.16 | 296.85 | 0.896 | 395.521 | | |
| 171 | 1579 | 9/13/2012 | 4 | 308.16 | 298.05 | 0.906 | 395.133 | | |
| 178 | 1579 | 9/24/2012 | 3 | 323.09 | 297.25 | 0.867 | 395.214 | | |
| 175 | 1579 | 9/15/2012 | 4 | 323.09 | 296.85 | 0.890 | 394.095 | 0.0123 g | 2.98E-03 |
| 167 | 1579 | 9/10/2012 | 7 | 323.09 | 296.45 | 0.903 | 395.521 | | |
| 170 | 1579 | 9/13/2012 | 3 | 323.14 | 297.85 | 0.913 | 395.133 | 0.0123 g | 3.04E-03 |

Table D.3: Experimental run information—additional parameters

| ID | Flow Rate (mL/min) | n | *a* (1/min) | $s_a$ | $R^2$ | use | $P_i^{sat}$ (Pa) | $B_{ii}$ (L/mol) | $\phi_i^{sat}$ |
|---|---|---|---|---|---|---|---|---|---|
| 116 | 40 | 8 | -2.976E-02 | 2.47E-04 | 1.000 | N | 3803.90 | -2.821 | 0.996 |
| 133 | 12 | 12 | -4.408E-03 | 8.43E-04 | 0.646 | N | 3803.90 | -2.821 | 0.996 |
| 135 | 40 | 24 | -2.204E-02 | 5.79E-04 | 0.985 | N | 3803.90 | -2.821 | 0.996 |
| 123 | 12 | 18 | -3.290E-03 | 3.49E-04 | 0.847 | N | 3803.90 | -2.821 | 0.996 |
| 126 | 40 | 18 | -1.275E-02 | 2.12E-04 | 0.996 | N | 3803.90 | -2.821 | 0.996 |
| 117 | 20.6 | 10 | -1.152E-02 | 3.25E-04 | 0.994 | Y | 3803.90 | -2.821 | 0.996 |
| 116 | 75 | 5 | -4.713E-02 | 2.66E-04 | 1.000 | Y | 3803.90 | -2.821 | 0.996 |
| 118 | 12 | 24 | -8.416E-03 | 7.31E-05 | 0.998 | Y | 3803.90 | -2.821 | 0.996 |
| 119 | 40 | 21 | -3.023E-02 | 2.39E-04 | 0.999 | Y | 3803.90 | -2.821 | 0.996 |
| 122 | 75 | 19 | -4.995E-02 | 4.31E-04 | 0.999 | Y | 3803.90 | -2.821 | 0.996 |
| 124 | 75 | 12 | -5.176E-02 | 2.93E-04 | 1.000 | Y | 3803.90 | -2.821 | 0.996 |
| 125 | 75 | 12 | -4.140E-02 | 3.75E-04 | 0.999 | Y | 3803.90 | -2.821 | 0.996 |
| 128 | 12 | 25 | -7.072E-03 | 1.43E-04 | 0.991 | Y | 3803.90 | -2.821 | 0.996 |
| 129 | 75 | 12 | -5.308E-02 | 2.28E-04 | 1.000 | Y | 3803.90 | -2.821 | 0.996 |
| 130 | 40 | 9 | -2.786E-02 | 4.30E-04 | 0.998 | Y | 3803.90 | -2.821 | 0.996 |
| 131 | 75 | 14 | -5.389E-02 | 1.77E-04 | 1.000 | Y | 3803.90 | -2.821 | 0.996 |
| 132 | 40 | 8 | -2.583E-02 | 7.31E-04 | 0.995 | Y | 3803.90 | -2.821 | 0.996 |
| 134 | 12 | 31 | -6.215E-03 | 2.57E-04 | 0.953 | Y | 3803.90 | -2.821 | 0.996 |
| 120 | 12 | 21 | -1.243E-02 | 8.79E-05 | 0.999 | Y | 6239.14 | -2.509 | 0.994 |
| 121 | 40 | 8 | -4.443E-02 | 1.04E-03 | 0.997 | Y | 6239.14 | -2.509 | 0.994 |
| 5 | 200 | 21 | -2.784E-04 | 2.18E-05 | 0.896 | Y | 900.84 | -10.036 | 0.996 |
| 2 | 200 | 27 | -4.328E-04 | 1.64E-05 | 0.965 | Y | 1797.89 | -7.800 | 0.995 |
| 4 | 200 | 21 | -5.840E-04 | 2.35E-05 | 0.970 | Y | 2487.26 | -6.906 | 0.993 |
| 1 | 200 | 29 | -1.163E-03 | 4.84E-05 | 0.955 | Y | 4580.99 | -5.459 | 0.991 |
| 3 | 200 | 21 | -1.063E-03 | 2.03E-05 | 0.993 | Y | 4580.99 | -5.459 | 0.991 |
| 103 | 200 | 19 | -2.935E-03 | 4.40E-04 | 0.723 | N | 150.11 | 0.000 | 1.000 |
| 107 | 200 | 14 | -2.095E-03 | 3.85E-04 | 0.712 | N | 150.22 | 0.000 | 1.000 |
| 92 | 200 | 19 | -4.867E-03 | 1.43E-04 | 0.986 | N | 348.35 | 0.000 | 1.000 |
| 89 | 200 | 24 | -4.429E-03 | 1.73E-04 | 0.967 | N | 348.81 | 0.000 | 1.000 |
| 88 | 200 | 20 | -4.693E-03 | 1.54E-04 | 0.981 | N | 349.74 | 0.000 | 1.000 |
| 101 | 200 | 14 | -3.084E-03 | 3.63E-05 | 0.998 | N | 150.00 | 0.000 | 1.000 |
| 102 | 200 | 13 | -2.576E-03 | 1.63E-04 | 0.958 | N | 150.00 | 0.000 | 1.000 |
| 108 | 200 | 21 | -2.468E-03 | 1.32E-04 | 0.949 | N | 150.00 | 0.000 | 1.000 |
| 100 | 200 | 16 | -3.128E-03 | 3.74E-04 | 0.833 | N | 150.11 | 0.000 | 1.000 |
| 111 | 200 | 44 | -2.334E-03 | 6.83E-05 | 0.965 | N | 150.33 | 0.000 | 1.000 |
| 113 | 200 | 29 | -2.378E-03 | 4.36E-05 | 0.991 | N | 150.33 | 0.000 | 1.000 |
| 115 | 200 | 24 | -2.350E-03 | 3.33E-05 | 0.996 | N | 150.33 | 0.000 | 1.000 |

Table D.3: Experimental run information—additional parameters (cont.)

| ID | Flow Rate (mL/min) | n | *a* (1/min) | $s_a$ | $R^2$ | use | $P_i^{sat}$ (Pa) | $B_{ii}$ (L/mol) | $\phi_i^{sat}$ |
|---|---|---|---|---|---|---|---|---|---|
| 109 | 200 | 29 | -2.655E-03 | 1.02E-04 | 0.962 | N | 150.55 | 0.000 | 1.000 |
| 90 | 125 | 20 | -3.397E-03 | 2.04E-04 | 0.939 | Y | 347.89 | 0.000 | 1.000 |
| 106 | 160 | 22 | -4.455E-03 | 1.58E-04 | 0.975 | Y | 348.35 | 0.000 | 1.000 |
| 93 | 160 | 21 | -4.422E-03 | 1.61E-04 | 0.975 | Y | 349.28 | 0.000 | 1.000 |
| 91 | 160 | 15 | -4.456E-03 | 2.13E-04 | 0.971 | Y | 349.74 | 0.000 | 1.000 |
| 112 | 160 | 28 | -4.538E-03 | 8.35E-05 | 0.991 | Y | 349.97 | 0.000 | 1.000 |
| 114 | 160 | 14 | -4.907E-03 | 6.49E-05 | 0.998 | Y | 350.20 | 0.000 | 1.000 |
| 99 | 160 | 19 | -8.650E-03 | 2.49E-04 | 0.986 | Y | 888.17 | 0.000 | 1.000 |
| 105 | 160 | 13 | -9.745E-03 | 2.68E-04 | 0.992 | Y | 889.74 | 0.000 | 1.000 |
| 97 | 160 | 20 | -9.316E-03 | 2.09E-04 | 0.991 | Y | 891.31 | 0.000 | 1.000 |
| 104 | 160 | 13 | -9.818E-03 | 2.94E-04 | 0.990 | Y | 892.35 | 0.000 | 1.000 |
| 96 | 125 | 16 | -1.460E-02 | 4.03E-04 | 0.989 | Y | 2016.78 | 0.000 | 1.000 |
| 98 | 125 | 15 | -1.583E-02 | 3.49E-04 | 0.994 | Y | 2019.96 | 0.000 | 1.000 |
| 94 | 160 | 13 | -1.955E-02 | 5.63E-04 | 0.991 | Y | 2021.02 | 0.000 | 1.000 |
| 110 | 160 | 15 | -1.878E-02 | 2.57E-04 | 0.998 | Y | 2021.02 | 0.000 | 1.000 |
| 95 | 125 | 12 | -1.568E-02 | 4.11E-04 | 0.993 | Y | 2022.08 | 0.000 | 1.000 |
| 35 | 80 | 11 | -3.950E-02 | 1.24E-03 | 0.991 | N | 7140.67 | -3.173 | 0.991 |
| 40 | 80 | 6 | -5.569E-02 | 8.70E-04 | 0.999 | N | 7140.67 | -3.173 | 0.991 |
| 38 | 12 | 16 | -7.035E-03 | 1.35E-04 | 0.995 | N | 7140.67 | -3.173 | 0.991 |
| 39 | 60 | 11 | -4.440E-02 | 1.69E-04 | 1.000 | N | 7140.67 | -3.173 | 0.991 |
| 59 | 60 | 12 | -4.460E-02 | 1.47E-04 | 1.000 | N | 7140.67 | -3.173 | 0.991 |
| 57 | 80 | 10 | -5.260E-02 | 4.99E-04 | 0.999 | N | 7140.67 | -3.173 | 0.991 |
| 61 | 80 | 7 | -6.091E-02 | 3.93E-04 | 1.000 | N | 7151.17 | -3.172 | 0.991 |
| 62 | 60 | 11 | -4.696E-02 | 1.30E-04 | 1.000 | N | 7151.17 | -3.172 | 0.991 |
| 33 | 12 | 14 | -7.577E-03 | 2.81E-04 | 0.984 | N | 7210.90 | -3.164 | 0.991 |
| 41 | 12 | 14 | -7.064E-03 | 1.78E-04 | 0.992 | N | 7210.90 | -3.164 | 0.991 |
| 34 | 60 | 16 | -4.461E-02 | 4.44E-04 | 0.999 | N | 7210.90 | -3.164 | 0.991 |
| 36 | 80 | 10 | -5.924E-02 | 4.28E-04 | 1.000 | N | 7210.90 | -3.164 | 0.991 |
| 50 | 40 | 13 | -3.719E-02 | 1.18E-03 | 0.989 | N | 11441.31 | -2.762 | 0.988 |
| 47 | 40 | 13 | -6.564E-02 | 1.35E-03 | 0.995 | N | 17530.56 | -2.434 | 0.984 |
| 44 | 40 | 10 | -7.455E-02 | 2.09E-03 | 0.994 | N | 21787.89 | -2.282 | 0.982 |
| 45 | 40 | 11 | -3.209E-02 | 3.85E-03 | 0.886 | N | 21787.89 | -2.282 | 0.982 |
| 58 | 20 | 12 | -1.674E-02 | 1.21E-04 | 0.999 | Y | 7133.68 | -3.174 | 0.991 |
| 60 | 20 | 9 | -1.655E-02 | 3.02E-04 | 0.997 | Y | 7137.18 | -3.174 | 0.991 |
| 37 | 40 | 10 | -3.179E-02 | 2.55E-04 | 0.999 | Y | 7140.67 | -3.173 | 0.991 |
| 32 | 40 | 20 | -3.322E-02 | 1.83E-04 | 0.999 | Y | 7210.90 | -3.164 | 0.991 |
| 51 | 40 | 10 | -5.333E-02 | 4.79E-04 | 0.999 | Y | 11389.49 | -2.765 | 0.988 |

Table D.3: Experimental run information—additional parameters (cont.)

| ID | Flow Rate (mL/min) | n | *a* (1/min) | $s_a$ | $R^2$ | use | $P_i^{sat}$ (Pa) | $B_{ii}$ (L/mol) | $\phi_i^{sat}$ |
|---|---|---|---|---|---|---|---|---|---|
| 42 | 40 | 11 | -5.131E-02 | 3.25E-04 | 1.000 | Y | 11441.31 | -2.762 | 0.988 |
| 43 | 40 | 11 | -4.992E-02 | 4.92E-04 | 0.999 | Y | 11441.31 | -2.762 | 0.988 |
| 52 | 40 | 10 | -7.685E-02 | 5.57E-04 | 1.000 | Y | 17523.17 | -2.434 | 0.984 |
| 48 | 40 | 10 | -7.620E-02 | 6.40E-04 | 0.999 | Y | 17530.56 | -2.434 | 0.984 |
| 53 | 40 | 8 | -7.298E-02 | 6.26E-04 | 1.000 | Y | 17545.37 | -2.433 | 0.984 |
| 54 | 40 | 7 | -7.877E-02 | 1.20E-03 | 0.999 | Y | 21471.13 | -2.292 | 0.982 |
| 55 | 40 | 10 | -9.078E-02 | 7.59E-04 | 0.999 | Y | 21497.39 | -2.291 | 0.982 |
| 56 | 40 | 10 | -8.442E-02 | 1.29E-03 | 0.998 | Y | 21506.14 | -2.291 | 0.982 |
| 46 | 40 | 11 | -9.225E-02 | 7.88E-04 | 0.999 | Y | 21611.45 | -2.288 | 0.982 |
| 49 | 40 | 7 | -9.020E-02 | 1.10E-03 | 0.999 | Y | 21699.52 | -2.285 | 0.982 |
| 62.5 | 40 | 12 | -4.826E-03 | 6.46E-04 | 0.848 | N | 11.25 | 0.000 | 1.000 |
| 82 | 60 | 30 | -2.853E-03 | 9.86E-05 | 0.968 | Y | 3.43 | 0.000 | 1.000 |
| 83 | 80 | 29 | -3.674E-03 | 1.01E-04 | 0.980 | Y | 3.44 | 0.000 | 1.000 |
| 84 | 80 | 27 | -3.503E-03 | 2.07E-04 | 0.919 | Y | 3.44 | 0.000 | 1.000 |
| 86 | 80 | 29 | -3.857E-03 | 6.77E-05 | 0.992 | Y | 3.44 | 0.000 | 1.000 |
| 85 | 80 | 27 | -3.613E-03 | 1.13E-04 | 0.976 | Y | 3.45 | 0.000 | 1.000 |
| 68 | 120 | 13 | -1.082E-02 | 2.77E-04 | 0.993 | Y | 10.93 | 0.000 | 1.000 |
| 67 | 40 | 16 | -5.050E-03 | 1.72E-04 | 0.984 | Y | 11.09 | 0.000 | 1.000 |
| 65 | 80 | 16 | -8.354E-03 | 1.99E-04 | 0.992 | Y | 11.25 | 0.000 | 1.000 |
| 66 | 120 | 13 | -1.215E-02 | 3.03E-04 | 0.993 | Y | 11.26 | 0.000 | 1.000 |
| 69 | 80 | 16 | -8.347E-03 | 2.47E-04 | 0.988 | Y | 11.26 | 0.000 | 1.000 |
| 70 | 60 | 8 | -5.120E-03 | 1.48E-04 | 0.995 | Y | 11.26 | 0.000 | 1.000 |
| 63 | 60 | 13 | -6.519E-03 | 2.01E-04 | 0.990 | Y | 11.30 | 0.000 | 1.000 |
| 79 | 60 | 17 | -6.887E-03 | 2.21E-04 | 0.985 | Y | 11.36 | 0.000 | 1.000 |
| 71 | 60 | 27 | -1.734E-02 | 7.29E-05 | 1.000 | Y | 43.19 | 0.000 | 1.000 |
| 72 | 60 | 16 | -1.714E-02 | 1.85E-04 | 0.998 | Y | 43.19 | 0.000 | 1.000 |
| 73 | 60 | 12 | -1.528E-02 | 3.97E-04 | 0.993 | Y | 43.19 | 0.000 | 1.000 |
| 81 | 60 | 12 | -1.692E-02 | 3.14E-04 | 0.997 | Y | 43.49 | 0.000 | 1.000 |
| 80 | 60 | 14 | -1.826E-02 | 3.21E-04 | 0.996 | Y | 43.64 | 0.000 | 1.000 |
| 74 | 60 | 20 | -3.492E-02 | 1.84E-04 | 1.000 | Y | 143.60 | 0.000 | 1.000 |
| 75 | 60 | 11 | -3.028E-02 | 3.34E-04 | 0.999 | Y | 143.83 | 0.000 | 1.000 |
| 76 | 60 | 10 | -3.748E-02 | 5.15E-04 | 0.998 | Y | 144.95 | 0.000 | 1.000 |
| 77 | 60 | 10 | -3.525E-02 | 1.31E-03 | 0.989 | Y | 144.95 | 0.000 | 1.000 |
| 78 | 60 | 10 | -3.076E-02 | 8.36E-04 | 0.994 | Y | 144.95 | 0.000 | 1.000 |
| 31 | 40 | 9 | -8.788E-03 | 3.25E-04 | 0.990 | N | 113.95 | 0.000 | 1.000 |
| 10 | 20 | 13 | -7.729E-03 | 3.94E-04 | 0.972 | N | 331.94 | 0.000 | 1.000 |
| 20 | 40 | 12 | -4.311E-02 | 6.95E-04 | 0.997 | N | 755.72 | 0.000 | 1.000 |

Table D.3: Experimental run information—additional parameters (cont.)

| ID | Flow Rate (mL/min) | n | *a* (1/min) | $s_a$ | R$^2$ | use | $P_i^{sat}$ (Pa) | $B_{ii}$ (L/mol) | $\phi_i^{sat}$ |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 40 | 10 | -8.981E-03 | 1.44E-04 | 0.998 | Y | 113.45 | 0.000 | 1.000 |
| 27 | 40 | 13 | -9.041E-03 | 2.80E-04 | 0.990 | Y | 113.65 | 0.000 | 1.000 |
| 30 | 40 | 11 | -8.746E-03 | 2.31E-04 | 0.994 | Y | 114.24 | 0.000 | 1.000 |
| 29 | 40 | 12 | -1.248E-02 | 2.33E-04 | 0.997 | Y | 175.09 | 0.000 | 1.000 |
| 28 | 40 | 13 | -1.272E-02 | 3.23E-04 | 0.993 | Y | 175.24 | 0.000 | 1.000 |
| 25 | 40 | 20 | -1.392E-02 | 2.13E-04 | 0.996 | Y | 176.13 | 0.000 | 1.000 |
| 12 | 60 | 10 | -3.227E-02 | 3.12E-04 | 0.999 | Y | 331.56 | 0.000 | 1.000 |
| 17 | 60 | 9 | -3.249E-02 | 5.99E-04 | 0.998 | Y | 331.94 | 0.000 | 1.000 |
| 16 | 80 | 10 | -4.126E-02 | 3.83E-04 | 0.999 | Y | 332.14 | 0.000 | 1.000 |
| 8 | 40 | 10 | -2.260E-02 | 5.24E-04 | 0.996 | Y | 332.39 | 0.000 | 1.000 |
| 6 | 60 | 13 | -3.234E-02 | 2.20E-04 | 0.999 | Y | 332.52 | 0.000 | 1.000 |
| 9 | 80 | 8 | -4.429E-02 | 9.81E-04 | 0.997 | Y | 332.52 | 0.000 | 1.000 |
| 13 | 40 | 10 | -2.230E-02 | 4.79E-04 | 0.996 | Y | 332.52 | 0.000 | 1.000 |
| 15 | 40 | 11 | -2.152E-02 | 3.08E-04 | 0.998 | Y | 332.52 | 0.000 | 1.000 |
| 21 | 40 | 13 | -1.944E-02 | 2.94E-04 | 0.997 | Y | 332.52 | 0.000 | 1.000 |
| 7 | 20 | 11 | -1.182E-02 | 3.43E-04 | 0.992 | Y | 333.49 | 0.000 | 1.000 |
| 11 | 80 | 10 | -4.034E-02 | 2.68E-04 | 1.000 | Y | 333.49 | 0.000 | 1.000 |
| 14 | 20 | 10 | -1.095E-02 | 2.58E-04 | 0.996 | Y | 333.49 | 0.000 | 1.000 |
| 24 | 40 | 9 | -3.049E-02 | 5.47E-04 | 0.998 | Y | 579.48 | 0.000 | 1.000 |
| 18 | 40 | 12 | -3.559E-02 | 6.52E-04 | 0.997 | Y | 584.24 | 0.000 | 1.000 |
| 22 | 40 | 14 | -4.404E-02 | 4.81E-04 | 0.999 | Y | 755.32 | 0.000 | 1.000 |
| 19 | 40 | 12 | -4.385E-02 | 8.40E-04 | 0.996 | Y | 756.11 | 0.000 | 1.000 |
| 23 | 40 | 9 | -4.572E-02 | 1.06E-03 | 0.996 | Y | 756.51 | 0.000 | 1.000 |
| 136 | 160 | 28 | -2.983E-03 | 2.06E-04 | 0.890 | Y | 149.12 | 0.000 | 1.000 |
| 137 | 160 | 22 | -2.533E-03 | 2.91E-04 | 0.791 | Y | 149.23 | 0.000 | 1.000 |
| 138 | 160 | 29 | -2.308E-03 | 1.78E-04 | 0.862 | Y | 149.01 | 0.000 | 1.000 |
| 139 | 160 | 25 | -2.492E-03 | 1.76E-04 | 0.897 | Y | 148.90 | 0.000 | 1.000 |
| 140 | 160 | 21 | -2.431E-03 | 1.55E-04 | 0.928 | Y | 149.01 | 0.000 | 1.000 |
| 141 | 40 | 17 | -5.297E-03 | 1.42E-04 | 0.989 | Y | 11.25 | 0.000 | 1.000 |
| 142 | 20 | 19 | -2.734E-03 | 5.46E-05 | 0.993 | Y | 11.23 | 0.000 | 1.000 |
| 143 | 40 | 11 | -2.529E-02 | 6.12E-04 | 0.995 | Y | 146.19 | 0.000 | 1.000 |
| 144 | 40 | 13 | -2.454E-02 | 2.35E-04 | 0.999 | Y | 146.87 | 0.000 | 1.000 |
| 145 | 40 | 6 | -2.922E-02 | 1.41E-03 | 0.991 | Y | 146.31 | 0.000 | 1.000 |
| 146 | 40 | 15 | -1.025E-02 | 1.55E-04 | 0.997 | Y | 43.27 | 0.000 | 1.000 |
| 147 | 40 | 27 | -1.862E-03 | 7.83E-05 | 0.958 | Y | 3.40 | 0.000 | 1.000 |
| 148 | 40 | 19 | -4.912E-03 | 1.59E-04 | 0.982 | Y | 11.23 | 0.000 | 1.000 |
| 149 | 20 | 23 | -1.325E-03 | 4.75E-05 | 0.974 | Y | 3.40 | 0.000 | 1.000 |

Table D.3: Experimental run information—additional parameters (cont.)

| ID | Flow Rate (mL/min) | n | $a$ (1/min) | $s_a$ | $R^2$ | use | $P_i^{sat}$ (Pa) | $B_{ii}$ (L/mol) | $\phi_i^{sat}$ |
|---|---|---|---|---|---|---|---|---|---|
| 150 | 20 | 22 | -1.319E-03 | 5.88E-05 | 0.962 | Y | 3.40 | 0.000 | 1.000 |
| 151 | 20 | 21 | -1.127E-03 | 6.26E-05 | 0.947 | Y | 3.41 | 0.000 | 1.000 |
| 177 | 40 | 5 | -1.223E-01 | 1.29E-02 | 0.968 | N | 312.47 | 0.000 | 1.000 |
| 165 | 60 | 17 | -9.249E-03 | 1.87E-04 | 0.994 | Y | 16.21 | 0.000 | 1.000 |
| 176 | 60 | 18 | -8.918E-03 | 2.70E-04 | 0.986 | Y | 16.27 | 0.000 | 1.000 |
| 178 | 60 | 23 | -8.111E-03 | 1.89E-04 | 0.989 | Y | 16.24 | 0.000 | 1.000 |
| 174 | 60 | 29 | -5.586E-03 | 1.27E-04 | 0.986 | Y | 16.28 | 0.000 | 1.000 |
| 158 | 20 | 21 | -6.145E-03 | 1.79E-04 | 0.984 | Y | 42.14 | 0.000 | 1.000 |
| 154 | 20 | 19 | -7.578E-03 | 1.83E-04 | 0.990 | Y | 42.17 | 0.000 | 1.000 |
| 163 | 20 | 17 | -4.762E-03 | 2.01E-04 | 0.974 | Y | 42.21 | 0.000 | 1.000 |
| 160 | 40 | 12 | -1.257E-02 | 4.26E-04 | 0.989 | Y | 42.08 | 0.000 | 1.000 |
| 157 | 40 | 15 | -1.141E-02 | 2.50E-04 | 0.994 | Y | 42.14 | 0.000 | 1.000 |
| 159 | 40 | 9 | -1.426E-02 | 3.49E-04 | 0.996 | Y | 42.14 | 0.000 | 1.000 |
| 161 | 40 | 11 | -1.197E-02 | 2.98E-04 | 0.994 | Y | 42.21 | 0.000 | 1.000 |
| 173 | 60 | 8 | -1.530E-02 | 3.84E-04 | 0.996 | Y | 42.08 | 0.000 | 1.000 |
| 155 | 60 | 9 | -2.187E-02 | 1.09E-03 | 0.983 | Y | 42.11 | 0.000 | 1.000 |
| 153 | 60 | 12 | -2.201E-02 | 2.30E-04 | 0.999 | Y | 42.14 | 0.000 | 1.000 |
| 162 | 60 | 11 | -1.915E-02 | 4.05E-04 | 0.996 | Y | 42.14 | 0.000 | 1.000 |
| 156 | 80 | 13 | -2.657E-02 | 2.49E-04 | 0.999 | Y | 42.08 | 0.000 | 1.000 |
| 152 | 80 | 12 | -2.897E-02 | 3.54E-04 | 0.999 | Y | 42.17 | 0.000 | 1.000 |
| 164 | 80 | 12 | -1.974E-02 | 2.16E-04 | 0.999 | Y | 42.24 | 0.000 | 1.000 |
| 172 | 40 | 12 | -2.513E-02 | 2.43E-04 | 0.999 | Y | 121.81 | 0.000 | 1.000 |
| 168 | 60 | 9 | -2.597E-02 | 2.21E-04 | 0.999 | Y | 121.89 | 0.000 | 1.000 |
| 169 | 60 | 6 | -3.236E-02 | 8.08E-04 | 0.998 | Y | 121.89 | 0.000 | 1.000 |
| 166 | 60 | 7 | -4.541E-02 | 6.52E-04 | 0.999 | Y | 121.97 | 0.000 | 1.000 |
| 171 | 60 | 6 | -4.801E-02 | 1.18E-03 | 0.998 | Y | 121.97 | 0.000 | 1.000 |
| 178 | 20 | 7 | -2.992E-02 | 1.08E-03 | 0.994 | Y | 312.47 | 0.000 | 1.000 |
| 175 | 40 | 7 | -7.261E-02 | 9.32E-04 | 0.999 | Y | 312.47 | 0.000 | 1.000 |
| 167 | 60 | 6 | -7.037E-02 | 3.04E-03 | 0.993 | Y | 312.47 | 0.000 | 1.000 |
| 170 | 60 | 5 | -1.106E-01 | 3.08E-03 | 0.998 | Y | 313.40 | 0.000 | 1.000 |

Table D.4: Experimental run calculated values

| ID | $\Psi$ | $s_{\Psi}$ | $\gamma_i^{\infty}$ | $s_{\gamma\infty}$ (%) | $k_H$ (kPa·mol/mol) | $s_{kH}$ (%) |
|---|---|---|---|---|---|---|
| 116 | 1 | 0 | 9.65E+03 | 5.2% | 3.66E+04 | 7.9% |
| 133 | 1 | 0 | 5.09E+03 | 5.2% | 1.93E+04 | 19.3% |
| 135 | 1 | 0 | 7.67E+03 | 5.2% | 2.90E+04 | 8.0% |
| 123 | 1 | 0 | 3.78E+03 | 5.2% | 1.43E+04 | 10.8% |
| 126 | 1 | 0 | 4.41E+03 | 5.2% | 1.67E+04 | 7.7% |
| 117 | 1 | 0 | 7.18E+03 | 5.2% | 2.72E+04 | 15.3% |
| 116 | 1 | 0 | 8.04E+03 | 5.2% | 3.05E+04 | 4.2% |
| 118 | 1 | 0 | 9.17E+03 | 5.2% | 3.47E+04 | 2.0% |
| 119 | 1 | 0 | 9.92E+03 | 5.2% | 3.76E+04 | 7.8% |
| 122 | 1 | 0 | 9.28E+03 | 5.2% | 3.52E+04 | 4.2% |
| 124 | 1 | 0 | 9.62E+03 | 5.2% | 3.64E+04 | 4.1% |
| 125 | 1 | 0 | 7.69E+03 | 5.2% | 2.91E+04 | 4.2% |
| 128 | 1 | 0 | 8.19E+03 | 5.2% | 3.10E+04 | 2.6% |
| 129 | 1 | 0 | 9.88E+03 | 5.2% | 3.74E+04 | 4.1% |
| 130 | 1 | 0 | 9.71E+03 | 5.2% | 3.68E+04 | 7.8% |
| 131 | 1 | 0 | 1.00E+04 | 5.2% | 3.80E+04 | 4.1% |
| 132 | 1 | 0 | 8.99E+03 | 5.2% | 3.41E+04 | 8.1% |
| 134 | 1 | 0 | 7.20E+03 | 5.2% | 2.73E+04 | 4.5% |
| 120 | 1 | 0 | 8.49E+03 | 5.2% | 5.26E+04 | 2.0% |
| 121 | 1 | 0 | 9.13E+03 | 5.2% | 5.66E+04 | 7.9% |
| 5 | 1 | 0 | 7.74E+01 | 25.3% | 6.94E+01 | 8.0% |
| 2 | 1 | 0 | 5.89E+01 | 25.2% | 1.05E+02 | 4.1% |
| 4 | 1 | 0 | 5.65E+01 | 25.2% | 1.40E+02 | 4.3% |
| 1 | 1 | 0 | 6.16E+01 | 25.1% | 2.80E+02 | 4.4% |
| 3 | 1 | 0 | 5.33E+01 | 25.1% | 2.42E+02 | 2.4% |
| 103 | 1 | 0 | 5.16E+03 | 25.4% | 7.74E+02 | 15.1% |
| 107 | 1 | 0 | 3.67E+03 | 25.4% | 5.51E+02 | 18.4% |
| 92 | 1 | 0 | 3.66E+03 | 25.4% | 1.27E+03 | 3.3% |
| 89 | 1 | 0 | 3.37E+03 | 25.4% | 1.18E+03 | 4.2% |
| 88 | 1 | 0 | 3.57E+03 | 25.4% | 1.25E+03 | 3.6% |
| 101 | 1 | 0 | 5.43E+03 | 25.4% | 8.14E+02 | 2.0% |
| 102 | 1 | 0 | 4.53E+03 | 25.4% | 6.80E+02 | 6.5% |
| 108 | 1 | 0 | 4.34E+03 | 25.4% | 6.51E+02 | 5.6% |
| 100 | 1 | 0 | 5.51E+03 | 25.4% | 8.28E+02 | 12.1% |
| 111 | 1 | 0 | 4.10E+03 | 25.4% | 6.17E+02 | 3.3% |
| 113 | 1 | 0 | 4.18E+03 | 25.4% | 6.28E+02 | 2.4% |

Table D.4: Experimental run calculated values (cont.)

| ID | $\Psi$ | $s_\Psi$ | $\gamma_i^\infty$ | $s_{\gamma\infty}$ (%) | $k_H$ (kPa·mol/mol) | $s_{kH}$ (%) |
|---|---|---|---|---|---|---|
| 115 | 1 | 0 | 4.13E+03 | 25.4% | 6.21E+02 | 2.1% |
| 109 | 1 | 0 | 4.65E+03 | 25.4% | 7.00E+02 | 4.1% |
| 90 | 1 | 0 | 4.09E+03 | 25.4% | 1.42E+03 | 6.5% |
| 106 | 1 | 0 | 4.15E+03 | 25.4% | 1.45E+03 | 4.0% |
| 93 | 1 | 0 | 4.15E+03 | 25.4% | 1.45E+03 | 4.1% |
| 91 | 1 | 0 | 4.16E+03 | 25.4% | 1.46E+03 | 5.1% |
| 112 | 1 | 0 | 4.23E+03 | 25.4% | 1.48E+03 | 2.7% |
| 114 | 1 | 0 | 4.58E+03 | 25.4% | 1.60E+03 | 2.3% |
| 99 | 1 | 0 | 3.07E+03 | 25.4% | 2.73E+03 | 3.4% |
| 105 | 1 | 0 | 3.44E+03 | 25.4% | 3.06E+03 | 3.3% |
| 97 | 1 | 0 | 3.29E+03 | 25.4% | 2.93E+03 | 2.9% |
| 104 | 1 | 0 | 3.46E+03 | 25.4% | 3.08E+03 | 3.5% |
| 96 | 1 | 0 | 2.71E+03 | 25.4% | 5.47E+03 | 3.5% |
| 98 | 1 | 0 | 2.93E+03 | 25.4% | 5.93E+03 | 3.1% |
| 94 | 1 | 0 | 2.86E+03 | 25.4% | 5.77E+03 | 3.4% |
| 110 | 1 | 0 | 2.74E+03 | 25.4% | 5.54E+03 | 2.2% |
| 95 | 1 | 0 | 2.92E+03 | 25.4% | 5.90E+03 | 3.4% |
| 35 | 1 | 0 | 3.67E+03 | 10.0% | 2.60E+04 | 5.0% |
| 40 | 1 | 0 | 5.20E+03 | 10.0% | 3.68E+04 | 4.2% |
| 38 | 1 | 0 | 4.36E+03 | 10.0% | 3.09E+04 | 2.5% |
| 39 | 1 | 0 | 5.53E+03 | 10.0% | 3.91E+04 | 5.1% |
| 59 | 1 | 0 | 5.56E+03 | 10.0% | 3.93E+04 | 5.1% |
| 57 | 1 | 0 | 4.91E+03 | 10.0% | 3.48E+04 | 4.0% |
| 61 | 1 | 0 | 5.68E+03 | 10.0% | 4.03E+04 | 3.9% |
| 62 | 1 | 0 | 5.84E+03 | 10.0% | 4.14E+04 | 5.1% |
| 33 | 1 | 0 | 4.65E+03 | 10.0% | 3.32E+04 | 4.1% |
| 41 | 1 | 0 | 4.32E+03 | 10.0% | 3.08E+04 | 3.0% |
| 34 | 1 | 0 | 5.49E+03 | 10.0% | 3.93E+04 | 5.2% |
| 36 | 1 | 0 | 5.48E+03 | 10.0% | 3.92E+04 | 3.9% |
| 50 | 1 | 0 | 4.23E+03 | 10.0% | 4.78E+04 | 8.0% |
| 47 | 1 | 0 | 4.70E+03 | 9.9% | 8.11E+04 | 7.6% |
| 44 | 1 | 0 | 4.14E+03 | 9.9% | 8.86E+04 | 7.8% |
| 45 | 1 | 0 | 1.76E+03 | 9.9% | 3.76E+04 | 14.0% |
| 58 | 1 | 0 | 6.26E+03 | 10.0% | 4.43E+04 | 15.2% |
| 60 | 1 | 0 | 6.19E+03 | 10.0% | 4.38E+04 | 15.3% |
| 37 | 1 | 0 | 5.94E+03 | 10.0% | 4.20E+04 | 7.7% |

Table D.4: Experimental run calculated values (cont.)

| ID | $\Psi$ | $s_{\Psi}$ | $\gamma_i^{\infty}$ | $s_{\gamma\infty}$ (%) | $k_H$ (kPa·mol/mol) | $s_{kH}$ (%) |
|---|---|---|---|---|---|---|
| 32 | 1 | 0 | 6.14E+03 | 10.0% | 4.39E+04 | 7.7% |
| 51 | 1 | 0 | 6.14E+03 | 10.0% | 6.91E+04 | 7.6% |
| 42 | 1 | 0 | 5.85E+03 | 10.0% | 6.61E+04 | 7.5% |
| 43 | 1 | 0 | 5.69E+03 | 10.0% | 6.43E+04 | 7.6% |
| 52 | 1 | 0 | 5.52E+03 | 9.9% | 9.52E+04 | 7.4% |
| 48 | 1 | 0 | 5.47E+03 | 9.9% | 9.43E+04 | 7.4% |
| 53 | 1 | 0 | 5.24E+03 | 9.9% | 9.05E+04 | 7.5% |
| 54 | 1 | 0 | 4.48E+03 | 9.9% | 9.44E+04 | 7.5% |
| 55 | 1 | 0 | 5.17E+03 | 9.9% | 1.09E+05 | 7.5% |
| 56 | 1 | 0 | 4.80E+03 | 9.9% | 1.01E+05 | 7.6% |
| 46 | 1 | 0 | 5.20E+03 | 9.9% | 1.10E+05 | 7.4% |
| 49 | 1 | 0 | 5.05E+03 | 9.9% | 1.08E+05 | 7.4% |
| 62.5 | 5.35E-01 | 4.49E-02 | 3.03E+02 | 6.7% | 6.37E+03 | 15.4% |
| 82 | 4.41E-01 | 6.23E-02 | 3.26E+02 | 8.0% | 2.54E+03 | 6.3% |
| 83 | 4.41E-01 | 6.23E-02 | 3.14E+02 | 8.0% | 2.45E+03 | 4.8% |
| 84 | 4.41E-01 | 6.23E-02 | 3.00E+02 | 8.0% | 2.34E+03 | 7.1% |
| 86 | 4.41E-01 | 6.23E-02 | 3.30E+02 | 8.0% | 2.58E+03 | 4.3% |
| 85 | 4.41E-01 | 6.22E-02 | 3.08E+02 | 8.0% | 2.41E+03 | 5.0% |
| 68 | 5.33E-01 | 4.54E-02 | 2.33E+02 | 6.8% | 4.78E+03 | 3.6% |
| 67 | 5.34E-01 | 4.52E-02 | 3.21E+02 | 6.7% | 6.67E+03 | 8.3% |
| 65 | 5.35E-01 | 4.49E-02 | 2.63E+02 | 6.7% | 5.53E+03 | 4.5% |
| 66 | 5.36E-01 | 4.49E-02 | 2.56E+02 | 6.7% | 5.38E+03 | 3.6% |
| 69 | 5.36E-01 | 4.49E-02 | 2.62E+02 | 6.7% | 5.51E+03 | 4.8% |
| 70 | 5.36E-01 | 4.49E-02 | 2.14E+02 | 6.7% | 4.51E+03 | 5.8% |
| 63 | 5.36E-01 | 4.49E-02 | 2.73E+02 | 6.7% | 5.76E+03 | 5.9% |
| 79 | 5.36E-01 | 4.48E-02 | 2.85E+02 | 6.7% | 6.04E+03 | 6.0% |
| 71 | 7.03E-01 | 2.51E-02 | 2.40E+02 | 5.6% | 1.48E+04 | 4.9% |
| 72 | 7.03E-01 | 2.51E-02 | 2.36E+02 | 5.6% | 1.45E+04 | 5.0% |
| 73 | 7.03E-01 | 2.51E-02 | 2.11E+02 | 5.6% | 1.29E+04 | 5.5% |
| 81 | 7.04E-01 | 2.50E-02 | 2.31E+02 | 5.6% | 1.43E+04 | 5.2% |
| 80 | 7.05E-01 | 2.50E-02 | 2.49E+02 | 5.6% | 1.54E+04 | 5.2% |
| 74 | 9.43E-01 | 4.66E-03 | 1.81E+02 | 5.0% | 2.75E+04 | 4.7% |
| 75 | 9.44E-01 | 4.63E-03 | 1.56E+02 | 5.0% | 2.38E+04 | 4.8% |
| 76 | 9.46E-01 | 4.47E-03 | 1.91E+02 | 5.0% | 2.92E+04 | 4.9% |
| 77 | 9.46E-01 | 4.47E-03 | 1.79E+02 | 5.0% | 2.75E+04 | 6.0% |
| 78 | 9.46E-01 | 4.47E-03 | 1.56E+02 | 5.0% | 2.39E+04 | 5.4% |

## Table D.4: Experimental run calculated values (cont.)

| ID | $\Psi$ | $s_{\Psi}$ | $\gamma_i^{\infty}$ | $s_{\gamma\infty}$ (%) | $k_H$ (kPa·mol/mol) | $s_{kH}$ (%) |
|---|---|---|---|---|---|---|
| 31 | 8.70E-01 | 0.05172 | 8.93E+01 | 25.5% | 1.17E+04 | 8.5% |
| 10 | 1 | 0 | 5.93E+04 | 10.9% | 1.97E+04 | 15.4% |
| 20 | 1 | 0 | 6.76E+04 | 10.9% | 5.11E+04 | 7.2% |
| 26 | 8.69E-01 | 0.052071 | 9.11E+01 | 25.5% | 1.19E+04 | 7.8% |
| 27 | 8.70E-01 | 0.051931 | 9.16E+01 | 25.5% | 1.20E+04 | 8.2% |
| 30 | 8.71E-01 | 0.051509 | 8.84E+01 | 25.5% | 1.16E+04 | 8.1% |
| 29 | 9.64E-01 | 0.014676 | 9.02E+01 | 25.0% | 1.64E+04 | 7.8% |
| 28 | 9.64E-01 | 0.014598 | 9.19E+01 | 25.0% | 1.67E+04 | 7.9% |
| 25 | 9.66E-01 | 0.014126 | 1.00E+02 | 25.0% | 1.83E+04 | 7.7% |
| 12 | 1 | 0 | 8.31E+04 | 10.9% | 2.76E+04 | 5.0% |
| 17 | 1 | 0 | 8.31E+04 | 10.9% | 2.76E+04 | 5.2% |
| 16 | 1 | 0 | 7.92E+04 | 10.9% | 2.63E+04 | 3.8% |
| 8 | 1 | 0 | 8.69E+04 | 10.9% | 2.89E+04 | 7.7% |
| 6 | 1 | 0 | 8.30E+04 | 10.9% | 2.76E+04 | 5.0% |
| 9 | 1 | 0 | 8.48E+04 | 10.9% | 2.82E+04 | 4.3% |
| 13 | 1 | 0 | 8.56E+04 | 10.9% | 2.85E+04 | 7.6% |
| 15 | 1 | 0 | 8.27E+04 | 10.9% | 2.75E+04 | 7.5% |
| 21 | 1 | 0 | 7.48E+04 | 10.9% | 2.49E+04 | 7.5% |
| 7 | 1 | 0 | 9.06E+04 | 10.9% | 3.02E+04 | 14.9% |
| 11 | 1 | 0 | 7.75E+04 | 10.9% | 2.59E+04 | 3.7% |
| 14 | 1 | 0 | 8.39E+04 | 10.9% | 2.80E+04 | 14.8% |
| 24 | 1 | 0 | 6.43E+04 | 10.9% | 3.73E+04 | 7.3% |
| 18 | 1 | 0 | 7.41E+04 | 10.9% | 4.33E+04 | 7.3% |
| 22 | 1 | 0 | 6.91E+04 | 10.9% | 5.22E+04 | 7.1% |
| 19 | 1 | 0 | 6.88E+04 | 10.9% | 5.21E+04 | 7.3% |
| 23 | 1 | 0 | 7.17E+04 | 10.9% | 5.42E+04 | 7.5% |
| 136 | 1 | 0 | 6.54E+03 | 10.9% | 9.75E+02 | 7.2% |
| 137 | 1 | 0 | 5.56E+03 | 10.9% | 8.30E+02 | 11.7% |
| 138 | 1 | 0 | 5.07E+03 | 10.9% | 7.56E+02 | 8.0% |
| 139 | 1 | 0 | 5.49E+03 | 10.9% | 8.17E+02 | 7.3% |
| 140 | 1 | 0 | 5.34E+03 | 10.9% | 7.96E+02 | 6.7% |
| 141 | 5.35E-01 | 4.49E-02 | 3.34E+02 | 6.7% | 7.01E+03 | 8.1% |
| 142 | 5.35E-01 | 4.50E-02 | 3.44E+02 | 6.7% | 7.23E+03 | 15.4% |
| 143 | 9.48E-01 | 4.29E-03 | 1.93E+02 | 5.0% | 2.97E+04 | 7.4% |
| 144 | 9.49E-01 | 4.20E-03 | 1.86E+02 | 5.0% | 2.88E+04 | 7.0% |
| 145 | 9.48E-01 | 4.28E-03 | 2.23E+02 | 5.0% | 3.44E+04 | 8.5% |

Table D.4: Experimental run calculated values (cont.)

| ID | $\Psi$ | $s_{\Psi}$ | $\gamma_i^{\infty}$ | $s_{\gamma\infty}$ (%) | $k_H$ (kPa·mol/mol) | $s_{kH}$ (%) |
|---|---|---|---|---|---|---|
| 146 | 7.03E-01 | 2.51E-02 | 2.12E+02 | 5.6% | 1.30E+04 | 7.4% |
| 147 | 4.40E-01 | 6.24E-02 | 3.22E+02 | 8.0% | 2.49E+03 | 9.0% |
| 148 | 5.35E-01 | 4.49E-02 | 3.08E+02 | 6.7% | 6.46E+03 | 8.3% |
| 149 | 4.40E-01 | 6.25E-02 | 4.58E+02 | 8.0% | 3.54E+03 | 16.3% |
| 150 | 4.40E-01 | 6.24E-02 | 4.56E+02 | 8.0% | 3.52E+03 | 16.5% |
| 151 | 4.40E-01 | 6.24E-02 | 3.89E+02 | 8.0% | 3.01E+03 | 16.8% |
| 177 | 1 | 0 | 4.74E+05 | 10.9% | 1.48E+05 | 13.3% |
| 165 | 1 | 0 | 5.11E+05 | 10.9% | 8.29E+03 | 5.7% |
| 176 | 1 | 0 | 4.91E+05 | 10.9% | 7.99E+03 | 6.1% |
| 178 | 1 | 0 | 4.49E+05 | 10.9% | 7.28E+03 | 5.8% |
| 174 | 1 | 0 | 3.07E+05 | 10.9% | 5.00E+03 | 5.8% |
| 158 | 1 | 0 | 3.87E+05 | 10.9% | 1.63E+04 | 15.6% |
| 154 | 1 | 0 | 4.78E+05 | 10.9% | 2.01E+04 | 15.5% |
| 163 | 1 | 0 | 3.00E+05 | 10.9% | 1.26E+04 | 15.9% |
| 160 | 1 | 0 | 3.97E+05 | 10.9% | 1.67E+04 | 8.4% |
| 157 | 1 | 0 | 3.59E+05 | 10.9% | 1.51E+04 | 8.0% |
| 159 | 1 | 0 | 4.50E+05 | 10.9% | 1.89E+04 | 8.0% |
| 161 | 1 | 0 | 3.77E+05 | 10.9% | 1.59E+04 | 8.1% |
| 173 | 1 | 0 | 3.22E+05 | 10.9% | 1.36E+04 | 5.7% |
| 155 | 1 | 0 | 4.60E+05 | 10.9% | 1.94E+04 | 7.2% |
| 153 | 1 | 0 | 4.63E+05 | 10.9% | 1.95E+04 | 5.2% |
| 162 | 1 | 0 | 4.03E+05 | 10.9% | 1.70E+04 | 5.5% |
| 156 | 1 | 0 | 4.20E+05 | 10.9% | 1.77E+04 | 4.0% |
| 152 | 1 | 0 | 4.57E+05 | 10.9% | 1.93E+04 | 4.0% |
| 164 | 1 | 0 | 3.10E+05 | 10.9% | 1.31E+04 | 4.0% |
| 172 | 1 | 0 | 2.65E+05 | 10.9% | 3.23E+04 | 7.4% |
| 168 | 1 | 0 | 1.82E+05 | 10.9% | 2.21E+04 | 4.9% |
| 169 | 1 | 0 | 2.27E+05 | 10.9% | 2.76E+04 | 5.5% |
| 166 | 1 | 0 | 3.19E+05 | 10.9% | 3.89E+04 | 5.1% |
| 171 | 1 | 0 | 3.39E+05 | 10.9% | 4.13E+04 | 5.6% |
| 178 | 1 | 0 | 2.27E+05 | 10.9% | 7.09E+04 | 14.6% |
| 175 | 1 | 0 | 2.77E+05 | 10.9% | 8.66E+04 | 7.4% |
| 167 | 1 | 0 | 1.78E+05 | 10.9% | 5.57E+04 | 6.5% |
| 170 | 1 | 0 | 2.83E+05 | 10.9% | 8.86E+04 | 5.8% |

# Appendix E. Prediction Method Sample Calculations

## E.1 First-Order Group Contribution Method

### E.1.1. 1,2,4,5-Tetramethylbenzene

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ |
|---|---|---|---|
| $CH_3$ | 4·(3.67) | 4·3683 | 4·(-8.73) |
| $CH_{ar}$ | 2·(-0.65) | 2·1849 | 2·(-4.16) |
| $C_{ar}$ | 4·(-3.85) | 4·(-102) | 4·(0.05) |
| I(C-C) | 2·(-1.01) | 2·6047 | 2·(-19.2) |
| $Y^0$ | 7.95 | 0 | 0 |
| Total | 3.91 | 30116 | -81.44 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \mathrm{kPa} \cdot 55.5084 \frac{\mathrm{mol}}{\mathrm{mol}} \cdot \exp\left( \frac{3.91 \cdot 1000 \frac{\mathrm{J}}{\mathrm{mol}}}{8.3145 \frac{\mathrm{J}}{\mathrm{mol} \cdot \mathrm{K}} \cdot 298.15 \cdot \mathrm{K}} \right) = 2.723 \cdot 10^4 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = (30116 \cdot \mathrm{K}) \left( \frac{1}{298.15 \cdot \mathrm{K}} - \frac{1}{T} \right) + (-81.44) \left( \ln\left( \frac{T}{298.15 \cdot \mathrm{K}} \right) \right) + \ln\left( 2.723 \cdot 10^4 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}} \right).$$

### E.1.2. 2,2-Dimethylhexane

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ |
|---|---|---|---|
| $CH_3$ | 4·(3.67) | 4·3683 | 4·(-8.73) |
| $CH_2$ | 3·(0.70) | 3·2962 | 3·(-8.43) |
| C | 1·(-4.51) | 1·1203 | 1·(-8.1) |
| $Y^0$ | 7.95 | 0 | 0 |
| Total | 20.22 | 24821 | -68.31 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \text{kPa} \cdot 55.5084 \frac{\text{mol}}{\text{mol}} \cdot \exp\left( \frac{20.22 \cdot 1000 \frac{\text{J}}{\text{mol}}}{8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} \cdot 298.15 \cdot \text{K}} \right) = 1.961 \cdot 10^7 \cdot \text{kPa} \frac{\text{mol}}{\text{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = (24821 \cdot \text{K})\left( \frac{1}{298.15 \cdot \text{K}} - \frac{1}{T} \right) + (-68.31)\left( \ln\left( \frac{T}{298.15 \cdot \text{K}} \right) \right) + \ln\left( 1.961 \cdot 10^7 \cdot \text{kPa} \frac{\text{mol}}{\text{mol}} \right).$$

### E.1.3. Methyl ethyl ketone

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ |
|---|---|---|---|
| $CH_3$ | 2·(3.67) | 2·3683 | 2·(-8.73) |
| $CH_2$ | 1·(0.70) | 1·2962 | 1·(-8.43) |
| C=O (ketone) | 1·(-22.74) | 1·4520 | 1·(-4) |
| $Y^0$ | 7.95 | 0 | 0 |
| Total | -6.75 | 14848 | -29.89 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \mathrm{kPa} \cdot 55.5084 \frac{\mathrm{mol}}{\mathrm{mol}} \cdot \exp\left( \frac{-6.75 \cdot 1000 \frac{\mathrm{J}}{\mathrm{mol}}}{8.3145 \frac{\mathrm{J}}{\mathrm{mol} \cdot \mathrm{K}} \cdot 298.15 \cdot \mathrm{K}} \right) = 3.694 \cdot 10^2 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = (14848 \cdot \mathrm{K}) \left( \frac{1}{298.15 \cdot \mathrm{K}} - \frac{1}{T} \right) + (-68.31) \left( \ln\left( \frac{T}{298.15 \cdot \mathrm{K}} \right) \right) + \ln\left( 3.694 \cdot 10^2 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}} \right).$$

## E.2 Second-Order Group Contribution Method

### E.2.1. 3-Methyl-1-butanol

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ | $D$ |
|---|---|---|---|---|
| O-(C)(H) | 1·(-25.46) | 1·(0) | 1·(0) | - |
| C-(C)(H)$_2$(O) | 1·(0.77) | 1·22467 | 1·(-49.8) | - |
| C-(H)(C)$_3$ | 1·(-1.93) | 1·(-4267) | 1·(11.8) | - |
| C-(H)$_2$(C)$_2$ | 1·(0.68) | 1·868 | 1·(-1.89) | - |
| C-(H)$_3$(C) | 2·3.72 | 2·6820 | 2·(-18.6) | - |
| $Y^0$ | 7.95 | 0 | 0 | - |
| Total | -10.55 | 32708 | -77.09 | 0.7774 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \mathrm{kPa} \cdot 55.5084 \frac{\mathrm{mol}}{\mathrm{mol}} \cdot \exp\left( \frac{-10.55 \cdot 1000 \frac{\mathrm{J}}{\mathrm{mol}}}{8.3145 \frac{\mathrm{J}}{\mathrm{mol} \cdot \mathrm{K}} \cdot 298.15 \cdot \mathrm{K}} \right) = 79.76 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = 0.7774 \cdot \left[ (32708 \cdot \mathrm{K}) \left( \frac{1}{298.15 \cdot \mathrm{K}} - \frac{1}{T} \right) + (-77.09) \left( \ln\left( \frac{T}{298.15 \cdot \mathrm{K}} \right) \right) \right] + \ln\left( 79.76 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}} \right)$$

.

### E.2.2. Ethylbenzene

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ | $D$ |
|---|---|---|---|---|
| $C\text{-}(H)_2(C)(Cb)$ | 1·(1.02) | 1·19962 | 1·(-65) | - |
| $Cb\text{-}(C)(Cb)_2$ | 1·(-4.53) | 1·(-13358) | 1·45 | - |
| $Cb\text{-}(H)(Cb)_2$ | 5·(-0.6) | 5·1870 | 5·(-4.28) | - |
| $C\text{-}(H)_3(C)$ | 1·3.72 | 1·6820 | 1·(-18.6) | - |
| $Y^0$ | 7.95 | 0 | 0 | - |
| Total | 5.16 | 22774 | -60 | 1 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \text{kPa} \cdot 55.5084 \frac{\text{mol}}{\text{mol}} \cdot \exp\left( \frac{5.16 \cdot 1000 \frac{\text{J}}{\text{mol}}}{8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} \cdot 298.15 \cdot \text{K}} \right) = 4.509 \cdot 10^4 \cdot \text{kPa} \frac{\text{mol}}{\text{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = 1 \cdot \left[ (22774 \cdot \text{K}) \left( \frac{1}{298.15 \cdot \text{K}} - \frac{1}{T} \right) + (-60) \left( \ln\left( \frac{T}{298.15 \cdot \text{K}} \right) \right) \right] + \ln\left( 4.509 \cdot 10^4 \cdot \text{kPa} \frac{\text{mol}}{\text{mol}} \right).$$

### E.2.3. *n*-Butyl ethyl ether

Structural information and group contributions:

| Group | $n_i \cdot \Delta G^{\infty}_{hyd,i}$ (kJ/mol) | $n_i \cdot B_i$ (K) | $n_i \cdot C_i$ | $D$ |
|---|---|---|---|---|
| $O\text{-}(C)_2$ | 1·(-15.52) | 1·(-29379) | 1·(68.9) | - |
| $C\text{-}(C)(H)_2(O)$ | 2·(0.77) | 2·22467 | 2·(-49.8) | - |
| $C\text{-}(H)_2(C)_2$ | 2·(0.68) | 2·868 | 2·(-1.89) | - |
| $C\text{-}(H)_3(C)$ | 2·3.72 | 2·6820 | 2·(-18.6) | - |
| $[CH_3\text{-}CH_2\text{-}O\text{-}CH_2]$ corr | 1·(-1.42) | 1·1106 | 1·(-6) | - |
| $Y^0$ | 7.95 | 0 | 0 | - |
| Total | 1.35 | 32037 | -77.68 | 0.7774 |

Equation 7.2 is rearranged to solve for $k_{H,ref}$:

$$k_{H,ref} = 101.325 \cdot \mathrm{kPa} \cdot 55.5084 \frac{\mathrm{mol}}{\mathrm{mol}} \cdot \exp\left( \frac{1.35 \cdot 1000 \frac{\mathrm{J}}{\mathrm{mol}}}{8.3145 \frac{\mathrm{J}}{\mathrm{mol} \cdot \mathrm{K}} \cdot 298.15 \cdot \mathrm{K}} \right) = 9.696 \cdot 10^3 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}}.$$

The overall temperature-dependent equation for $k_H$ is predicted by:

$$\ln(k_H) = 0.7774 \cdot \left[ (32037 \cdot \mathrm{K}) \left( \frac{1}{298.15 \cdot \mathrm{K}} - \frac{1}{T} \right) + (-77.68) \left( \ln\left( \frac{T}{298.15 \cdot \mathrm{K}} \right) \right) \right] + \ln\left( 9.696 \cdot 10^3 \cdot \mathrm{kPa} \frac{\mathrm{mol}}{\mathrm{mol}} \right)$$