Developing High Precision Heat Capacity Correlations for Organic Solids and Liquids - Extending to Biofuels and Sugars

by

Jenny Boutros

A thesis submitted in partial fulfillment of the requirements for the degree of

Master of Science

in

Chemical Engineering

Department of Chemical and Materials Engineering
University of Alberta

Abstract

There is a great need for easily accessible and accurate physical property data in the heavy oil industry, the pharmaceutical industry, and other heavy molecule guided productions. In recent years, high precision predictive correlations for isobaric heat capacities of heavy and ill-defined organic solids, liquids and ideal gases have been developed by the petroleum thermodynamics research team at the University of Alberta. The Laštovka-Shaw and Dadgostar-Shaw correlations are based on the similarity variable concept, rooted in quantum mechanics. This concept is directly related to the routinely available elemental analysis, and is a solid foundation for further developing energy models.

In this work, we aimed to first develop chemical family specific isobaric heat capacity correlations for solid and liquid hydrocarbons based on the Laštovka-Shaw (solid) and Dadgostar-Shaw (liquid) correlations. Second, we aimed to extend the range of application for the two correlations to include heteroatom-rich bio-diesel (primarily liquids), and sugars (primarily solids).

For the development of family specific correlations, we relied on mathematical optimization of the correlation's universal coefficients, while preserving the same original functionality. Family specific forms were developed for solids: alkanes, alkenes, esters, and carboxylic acids; and for liquids: alkanes, naphthene, aromatic and unsaturated cyclics. As for the extension of the correlations, we introduced an adjusting parameter that is directly related to heteroatom weight percent. Laštovka-Shaw's correlation for solids was extended to sugars, and Dadgostar-Shaw's correlation for liquids was extended to biofuels, with an absolute average relative error in prediction at around 5%.

Published experimental and theoretical work indicate the need for optimizing methods for the estimation of isobaric heat capacity for various families and groups of compounds. Therefore, new modified forms of the Laštovka-Shaw and Dadgostar-Shaw correlations were presented, expanding the prediction of isobaric heat capacities to high heteroatom containing compounds. This work recommends an extension of these correlations to industrially relevant feed materials, like biofuels and sugars, and ultimately pharmaceuticals and biomedical products.

Acknowledgement

First, I would like to extend my thank you to Dr. John Shaw, for his unending patience during this long journey. He provided valuable assistance and advice whenever I needed it.

I would also like to acknowledge Mildred Becerra, Sourabh Ahitan and Linda Kaert for helping me edit this thesis, and for always helping me out around the office and the Lab.

Finally, my deepest thank you for my mom and dad, Georges, Michael, Gabriel, and Evan. Your support and continuous encouragement kept me going. Thank you, I love you.

Jenny Boutros

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

List of Symbols

c_p	Specific heat capacity at constant pressure, $J \cdot K^{-1} \cdot g^{-1}$
C_p	Molar heat capacity at constant pressure, $J \cdot K^{-1} \cdot mol^{-1}$
H	Enthalpy, J. mol^{-1}
T	Temperature, K
T_b	Normal boiling Temperature, K
spgr	Specific gravity, $g.cm^3$
M	Molar mass, $g \cdot mol^{-1}$
c_p^{g0}	Specific heat capacity of ideal gas at constant pressure, $J \cdot K^{-1} \cdot g^{-1}$
C_p^{g0}	Molar heat capacity of ideal gas at constant pressure, $J \cdot K^{-1} \cdot mol^{-1}$
θ	Einstein's temperature, K and adjustable fitting parameter
N	Number of atoms in a molecule
n_c	Carbon atom number
C_{pL}	Liquid heat capacity when enthalpy changes regarding temperature at constant pressure, $J \cdot K^{-1} \cdot mol^{-1}$
$C_{\sigma L}$	Liquid heat capacity when enthalpy of a saturated liquid changes regarding temperature at constant pressure, $J \cdot K^{-1} \cdot mol^{-1}$
C_{satL}	Liquid heat capacity when liquid is in a saturated state, $J \cdot K^{-1} \cdot mol^{-1}$

P	Pressure, Pa
$V_{\sigma L}$	Volume of a saturated liquid, when enthalpy is changing with respect to temperature, m^3
T_r	Reduced Temperature, K
P_c	Critical pressure, Pa
T_c	Critical temperature, K
ω	Acentric factor
$C_V^{translation}$	Contribution to the molar heat capacity at constant volume from the translational motion of a molecule as a whole, $J \cdot K^{-1} \cdot mol^{-1}$
$C_V^{rotation}$	Contribution to the molar heat capacity at constant volume from the rotational motion of a molecule as a whole, $J \cdot K^{-1} \cdot mol^{-1}$
$C_V^{vibration}$	Contribution to the molar heat capacity at constant volume from the intramolecular vibrations in a molecule, $J \cdot K^{-1} \cdot mol^{-1}$
R	Universal gas constant, $R = 8.314472\ J \cdot K^{-1} \cdot mol^{-1}$
h	Planck constant, $h = 6.62606957 \cdot 10^{-34}\ J \cdot s$
ϑ_i	Frequency of i^{th} intramolecular vibration, Hz
k_B	Boltzmann constant, $k_B = 1.3806488 \cdot 10^{-23}\ J \cdot K^{-1}$
$C_{p,linear}^{g0}$	Molar ideal gas heat capacity at constant pressure for linear molecules, $J \cdot K^{-1} \cdot mol^{-1}$
$C_{p,nonlinear}^{g0}$	Molar ideal gas heat capacity at constant pressure for non-linear molecules, $J \cdot K^{-1} \cdot mol^{-1}$
n	Number of elements in a compound and number of experimental data
f	Total number of vibration modes in a molecule

m	Mass of a molecule, g and number of compounds in a dataset
φ	Number of vibration modes per mass of a molecule, g^{-1}
N_A	Avogadro's number, N_A= 6.022140857.10^{-23} mol^{-1}
α	Similarity variable, $mol \cdot g^{-1}$
w_i	Mass fraction of element *i* in a compound, g
x_i	Mole fraction of element *i* in a compound, mol
v_i	Stoichiometric coefficient for element i in a compound
T_{sat}	Temperature of Saturation, K
$c_p^{g0,DFT}$	Computed DFT RRHO specific ideal gas heat capacity, $J \cdot K^{-1} \cdot g^{-1}$
$c_p^{g0,A}$	Computed DFT RRHO specific ideal gas heat capacity for compound A, $J \cdot K^{-1} \cdot g^{-1}$
$c_p^{g0,B}$	Computed DFT RRHO specific ideal gas heat capacity for compound B, $J \cdot K^{-1} \cdot g^{-1}$
c_{pLS}	Specific heat capacity of solid at constant pressure calculated using the Laštovka -Shaw correlation, $J \cdot K^{-1} \cdot g^{-1}$
c_{pALS}	Specific heat capacity of solid at constant pressure calculated using the adjusted Laštovka -Shaw correlation, $J \cdot K^{-1} \cdot g^{-1}$
c_{pDS}	Specific heat capacity of liquid at constant pressure calculated using the Dadgostar-Shaw correlation, $J \cdot K^{-1} \cdot g^{-1}$
c_{pADS}	Specific heat capacity of liquid at constant pressure calculated using the adjusted Dadgostar-Shaw correlation, $J \cdot K^{-1} \cdot g^{-1}$
C_p^s	Solid isobaric heat capacity, $J \cdot K^{-1} \cdot mol^{-1}$
C_p^l	Liquid isobaric heat capacity, $Btu.lb^{-1}$. deg R^{-1}

c_p^{exp}	Specific experimental isobaric heat capacity, $J \cdot K^{-1} \cdot g^{-1}$
c_p^{cal}	Correlation calculated specific isobaric heat capacity, $J \cdot K^{-1} \cdot g^{-1}$
K_w	Watson characterization factor = (mean average boiling point)$^{1/3}$/spgr
T_m	Melting point, K
w_{SNO}	Mass fraction of heteroatom in a compound, g
V	Volume, m^3
V_c	Critical volume, m^3
w_O	Mass fraction of oxygen in a compound, g
δ	Average absolute deviation, $J \cdot K^{-1} \cdot g^{-1}$
ε	Average absolute relative deviation, $J \cdot K^{-1} \cdot g^{-1}$
$c_{p,sample}$	Solid heat capacity at constant pressure of a sugar sample measured using the differential scanning calorimeter (DSC), $J \cdot {}^oC^{-1} \cdot g^{-1}$
$c_{p,sapphire}$	Solid heat capacity at constant pressure of a sapphire sample measured using the differential scanning calorimeter (DSC), $J \cdot {}^oC^{-1} \cdot g^{-1}$
HF_{blank}	Heat flow of a blank sample in the (DSC), $J.s^{-1}$
$HF_{sapphire}$	Heat flow of a sapphire sample in the (DSC), $J.s^{-1}$
HF_{sample}	Heat flow of a sugar sample in the (DSC), $J.s^{-1}$
$N_{frag,A}$	Number of fatty acid fragments
$C_{p,A}^l$	Liquid heat capacity of a fatty acid fragment, $J \cdot K^{-1} \cdot mol^{-1}$
$C_{p,FA}^l$	Liquid heat capacity of a fatty acid, $J \cdot K^{-1} \cdot mol^{-1}$
C_{pi}^l	Liquid heat capacity of a specific chemical group, $J \cdot K^{-1} \cdot mol^{-1}$

C_{pi}^{o}	Ideal gas heat capacity of a specific chemical group, $J \cdot K^{-1} \cdot mol^{-1}$
$C_{p,FA}^{o}$	Ideal gas heat capacity of a fatty acid, $J \cdot K^{-1} \cdot mol^{-1}$
$C_{p,est}$	Estimated liquid heat capacity, $J \cdot K^{-1} \cdot mol^{-1}$
N_k	Number of different groups on a molecule
ω_i	Acentric factor of a specific fatty acid group
ω_{mix}	Acentric factor of a fatty acid mixture
$T_{c,i}$	Critical temperature of a specific fatty acid group, K
$T_{c,mix}$	Critical temperature of a fatty acid mixture, K
F_c	Heat capacity correction factor, $J \cdot K^{-1} \cdot mol^{-1}$
S	Objective function to be minimized
$a_{1,2,3}$, a, b, c, d, e, f, G, $A_{1,2,3}$, B_{11}, B_{12}, B_{21}, B_{22}, C_{11}, C_{12}, C_{21}, C_{22}, a_{11}, a_{12}, a_{21}, a_{22}, a_{31}, a_{32}, A, θ, C_1, C_2, D_1, D_2, A_k, B_k, $A_{1,A}$, $A_{2,A}$	Adjustable coefficients of fitting equations

1 Introduction

1.1 The Basics of Constant Pressure Heat Capacity Calculations

One of the most important characteristics of a compound is its constant pressure heat capacity (c_p). In thermodynamics, heat capacity is used to calculate entropy and enthalpy values, in thermochemistry, it is used to measure the change in enthalpy of reactions at different temperatures, and in chemical engineering, it is widely used for writing energy balances. Moreover, heat capacity is essential for evaluating the effect of temperature on phase and reaction equilibria. Observing variations in heat capacity with temperature serves as an indicator of phase and structure changes in both solids and liquids[1,2].

Heat capacity is evidently of great importance for the accurate calculation of other thermodynamic properties of real gases, liquids, and solids, as it is directly related to the temperature derivative of basic thermodynamic functions. Accurate values for heat capacities at constant pressure are essential for generating reliable data in the calculation of diverse thermodynamic properties when changes in temperature occur. Constant pressure heat capacity is defined as the following:

$$\boldsymbol{C_p = \left(\frac{\partial H}{\partial T}\right)_p} \tag{1-1}$$

Depending on the units used for the enthalpy (H), Equation (1-1) might represent either a molar ($\boldsymbol{C_p}$; $J \cdot K^{-1} \cdot mol^{-1}$) or specific heat capacity (c_p ; $J \cdot K^{-1} \cdot g^{-1}$) [3].

Many estimation techniques for solid and liquid isobaric heat capacities are available in open literature. For solids, the literature related to estimation methods is fragmented. In most cases, methods are based on knowledge of molecular structure or have only been designed for specific groups of organic compounds, or are only applicable to pure low molar mass compounds. Most of these methods are derived over a small range of temperatures and do not provide accurate estimates for ill-defined large molecules. Also for liquids, many estimation methods exist, but they pose similar problems as the ones for solids in that they often require detailed physical properties and molecular structures of the compounds at hand. Similarly, these methods are often derived for a specific family over a small range of temperatures and require prior knowledge of other thermophysical properties such as structures and critical temperatures. For pure hydrocarbon compounds and well-defined mixtures there are many data sets and compilations of data available through the National Institute of Standards and Technology (NIST - SRD 103b, SRD 4). At the other extreme, thermophysical data for heavy oils and their fractions are often not readily available, creating a need to develop strong predictive models based on minimal data and fewer input parameters. Some of these predictive techniques, for both solid and liquid isobaric heat capacity, will be discussed in more detail in Section 2.

The classification of conventional petroleum and other heavy oil mixtures into defined and undefined mixtures, has led to two different methods of characterization. When

dealing with a defined mixture, where molecular structures are known, the physical properties are often extrapolated from those of model compounds such as n-paraffin, naphthenic, and polyaromatics, following simple mixing rules. As for undefined mixtures or fractions, they are usually characterized as mixtures of pseudo-components using generalized empirical correlations, which are functions of boiling point (T_b) and specific gravity ($spgr$)[5]. For high molar mass fractions (M > 300 g·mol^{-1}), distillation data are typically not available, and this leads to the use of less well-defined input data and less accurate models that require significant tuning. For example, boiling point ranges for heavy ends are often obtained by correlating their retention times in a chromatographic column to n-alkane reference compounds.

In current practice, some of the most accurate heat capacity values for pure compounds are calculated using quantum mechanical methods. These quantum mechanical calculations are based on Density Functional Theory (DFT), and are used to calculate fundamental vibrations[6]. Usually, a simple Rigid Rotor-Harmonic Oscillated model (RRHO) is used as a first order approximation to determine the fundamental vibrations in a compound and then with the use of statistical thermodynamics, the heat capacity is calculated. However, values of high accuracy can only be obtained through introduction of scaling factors for computed vibration frequencies, and corrections for rotational-vibrational coupling, internal rotation, and centrifugal distortion[4,7]. In the case of large molecules and ill-defined hydrocarbon mixtures a detailed determination of the internal degrees of freedom becomes computationally intensive and infeasible, respectively. For typical engineering and

industrial calculations, significant uncertainties in average molecular structure arise, and therefore, quantum mechanical methods cannot be applied.

Recently, the thermodynamics research group at the University of Alberta has presented robust alternative predictive methods encompassing solid[8], liquid[9] and vapor[10] isobaric heat capacity estimation based on the similarity variable identified by Laštovka et al.[11]. These methods are valid for a wide range of hydrocarbons and they rely solely on knowledge of the elemental composition of a fluid or a class of fluids. Elemental analysis is a simple and inexpensive analysis that is readily and routinely performed in industry. The resulting correlations estimating isobaric heat capacities of solids (Laštovka-Shaw)[8] and liquids (Dadgostar-Shaw)[9] yielded average relative deviations in estimated isobaric heat capacity data below 10% suggesting that these correlations are suitable bases for developing high-precision fluid family-specific correlations. Family specific data can prove valuable for targeted productions, where an optimized form of the generic correlation can be used.

In the present work, high-precision predictive correlations for specific mixed fluids and families of compounds are obtained by tuning the first term of the Laštovka-Shaw and Dadgostar-Shaw universal correlations, while retaining their overall reliability. These high precision correlations lead to a reduction in prediction error for specific fluid families while avoiding the pitfalls found in other predictive methods ie. need for extensive physical properties. Moreover, this work attempts to extend the concept to other categories of compounds with high heteroatom content. Laštovka and Shaw[10]

determined that for hydrocarbons, the computed ideal gas isobaric heat capacity c_p^{g0}, is primarily a function of the number of vibrations per mass of a molecule. However, they observed small deviations in c_p^{g0} temperature dependence for compounds that possess the same value of the similarity variable i.e. same vibration per molecular mass, but different molecular structure (cyclic vs. acyclic aliphatic compounds). Larger deviations were also observed and discussed for compounds with high mass fractions of heteroatoms, Sulfur (S), Nitrogen (N), Oxygen (O), and they restricted the application of correlations to heteroatom mass fractions less than 0.15 [4]. Even though this limit covers a broad range of compound classes and petroleum fluids, these secondary effects related to structure and heteroatom content must be explored and resolved if generalizable isobaric heat capacity correlations are to be developed for food, biofuel and pharmaceutical applications where heteroatom mass fractions are typically well in excess of 0.15 and more typically closer to 0.5 [12].

1.2 Industrial Needs

Accurate thermophysical property characterizations of compounds and mixtures have direct positive effects on the techno-economic and environmental impact analyses for all the chemical process industries. Also, they are essential for the efficient planning, design and optimization of related industrial operations. Reliable isobaric heat capacity models for biofuels, sugars, and for related materials, are no exception. These materials differ in molecular structure, often being more naphthenic, and in elemental composition with higher oxygen content from typical hydrocarbons for which well-

tested heat capacity models with varying degrees of sophistication and complexity exist. A parallel set of accurate heat capacity models are needed for the bio-energy and bio-molecule sectors. The existing models underpinning engineering processes and product related calculations in the hydrocarbon energy and petrochemical sectors, provide poor heat capacity estimates for individual bio-molecules and for both simple and complex mixtures.

For example, the production of biodiesel, an important alternative fuel, requires a prior knowledge of thermophysical properties of biodiesel, and the materials used to produce it. Only in this way can the processes involved in production be selected, combined and operated optimally. The heat capacity of biodiesel impacts all the heat exchange operations. As with their fossil fuel analogues, these mixtures comprise potentially millions of individual compounds and heat capacity models must be based on black oil equivalent models with a comparable level of chemical analysis and fluid characterization. A common approach is to identify and to adapt models based on empirical equations and fluid characterization techniques developed for conventional hydrocarbons and ill-defined mixtures (outlined in section 1.1) to the emerging biomolecule equivalents.

Accurate and general-purpose heat capacity models are equally important for the pharmaceutical, and by extension, sugar industry where the ability to discriminate solid states, and solid-liquid transitions of individual compounds can be pivotal. In pharmaceutical industry, undesired states may have no therapeutic value or may be

toxic. Having robust models is also important for process design in this sector, where significant effort goes into the experimental evaluation of heat capacity and phase behaviour of individual compounds. Accurate but generic heat capacity models act as references for detecting differences including subtle solid-solid transitions. Again, it is apparent, that generic models based on simple characterization (elemental analysis, basic structural features) are required.

2 Literature review

2.1 Isobaric Heat Capacity Prediction Methods

Reliable and accurate estimation techniques are needed for estimating heat capacity, because of its importance in the design and integration of process units such as heat exchangers in the oil refining sector. Specific chemical families, structure details, low molar mass, or temperature ranges usually limit heat capacity estimation techniques. Their application to large compounds, and ill-defined mixtures, over the wide range of temperatures encountered in industry can prove challenging. Moreover, experimental heat capacity data are scarce for large compounds and industrially relevant mixtures. New high precision data are sorely needed for the creation, extension, and evaluation of isobaric heat capacity models.

2.1.1 Organic Solids

There are few available methods for solid state isobaric heat capacity prediction for organic compounds, and the data in the literature for large molecules are scarce. Group contribution methods, except for the method developed by Goodman et al.[13], are valid only at 298K[14,15,16]. These techniques were developed for low molar mass organic solids, however the Helgeson method[17] was later extended Richard and Helgeson[18] to include large organic compounds. There is also a method based on the sum of element contributions, valid only at 298K, that was developed by Hurst and Harrison[19]. The additive method of Kabo et al.[20] is valid in the temperature range 10 to 150 K, and it encompasses isobaric heat capacities of alkanes, alkenes, alkanols,

alkanones, alkyl and phenyl derivatives of urea[21]. Laštovka and Shaw[8] applied their similarity variable concept to solids and developed and validated their equation over a wide range of temperatures (50 K to melting temperature) for large molecules and poorly defined mixtures of organic solids. Their approach requires elemental analysis but does not require molecular structure knowledge. Table 2.1 shows a comparison of range and data required for common solid isobaric heat capacity prediction techniques with Laštovka and Shaw's correlation. With average absolute prediction errors below 10%, it is a strong candidate for the generation of accurate fluid family specific equations. Details regarding their similarity concept and their correlation are presented in section 2.2.

Table 2.1. Estimation Methods for Isobaric Solid Heat Capacity.

Estimation Method	Data Required	Method	Compound Range
Goodman et al.[13]	Molecular structure	GCM	Pure Compounds
Richard and Helgeson[18]	Molecular Structure	GCM	High MW HC, Ill-defined Mixtures
Hurst and Harrison[19]	Molecular Structure	Modified Kopp's Rule	Pure Compounds
Kabo et al.[20]	Molecular Structure	Additive Method	Pure Compounds
Briard et al.[22]	n_c, N, θ, T	Einstein's Model	n-Alkanes
Laštovka -Shaw[8]	Elemental Analysis	Similarity Variable	Wide range of HC, high MW HC, ill-defined mixtures

2.1.2 Organic Liquids

Before reviewing liquid phase isobaric heat capacity prediction methods, it is important to define the liquid heat capacity terms and definitions that are used in these different models. In 1965, Reid and Sobel[23], presented three definitions of liquid heat capacity, $C_{pL,}$ $C_{\sigma L}$, andC_{satL}. Predictive methods usually report C_{pL}, and $C_{\sigma L}$. Whereas C_{satL} are obtained experimentally:

- C_{pL}: Liquid heat capacity, when change in enthalpy is with respect to temperature under constant pressure
- $C_{\sigma L}$: Liquid heat capacity, when change in enthalpy of a saturated liquid is with respect to the temperature along the saturation curve
- C_{satL}: Liquid heat capacity, describing the amount of heat required to cause a change in the temperature, of a saturated liquid

The values of these three terms are indistinguishable at reduced temperatures (T_r) less than 0.8. However, these values differ greatly as critical points are approached[23]. The relationship between those terms is defined as[24]:

$$C_{\sigma L} = C_{pL} + \left[C_{\sigma L} - T\left(\frac{\partial V}{\partial T}\right)_p\right]\left(\frac{\partial V}{\partial T}\right)_{\sigma L} = C_{satL} - V_{\sigma L}\left(\frac{dP}{dT}\right)_{\sigma L} \quad (2\text{-}1)$$

Where, $V_{\sigma L}$ is the volume of a saturated liquid with respect to temperature along the saturation curve. Below is a brief discussion of some of the most widely used techniques for the prediction of liquid isobaric heat capacity.

***Group Contribution methods*:**

These methods rely on two main assumptions. First, that each molecular structure is made up of different groups vibrating independently from each other, and second, that each of these groups contributes a specific value to the total molar heat capacity (C_{pL}). Available methods are often limited by temperature range under which the correlation was developed, even when data they report show low deviations (in the range of two to three percent). Chueh and Swanson's[25,26] work is valid only at 293 K whereas, Missenard's[27,28] work is limited to a temperature range of T_r< 0.75 and for compounds without double bonds. Other available methods like the work done by Růžička and Domalski[29], take into consideration dissimilar contributions related to what an atom is bonded to. However, this method underestimated C_{pL} at high temperatures. These techniques cannot be used for ill-defined materials since they require extensive knowledge of molecular structure.

Corresponding States methods:

One of the most widely used correlations for calculating liquid heat capacity is the Lee-Kesler[30] correlation, a corresponding state method, which was also the basis for many other corresponding states techniques. Although this technique usually leads to good heat capacity estimates, it requires accurate critical temperature (T_c)

and critical pressure (P_c), and the acentric factor (ω) of the compound in question. The Lee-Kesler method is used in most engineering simulators as a default method for isobaric liquid heat capacity estimation approach even outside its range of application, where outcomes of variable quality are obtained. The Rowlinson-Bondi method[31,32] is valid for low values of T_r and for values approaching one. For this method C_p^{g0}, T_c, and ω are needed.

Thermodynamic cycle methods:

Reid and Sobel[23] introduced multiple expressions based on reduced saturated liquid density and compressibility factor differences between saturated vapor and liquid. However, the method of Tyagi[33] is the most prominent and accurate one. Even though it does not provide reliable results for mixtures and ill-defined fluids.

Thermodynamic models:

A lot of thermodynamic models are available for estimation of heat capacities of solids and liquids. These typically require knowledge of molecular structure, mean molar mass, reference heat capacity values and critical properties as inputs. These methods often work well for defined compounds and mixtures of small compounds, but start lacking in accuracy as molar mass increases[34]. Employing these methods for ill-defined hydrocarbons can prove challenging. Bessières et al.[35] have investigated the potential of thermodynamic models in the prediction of heavy cuts characteristic properties. Some of the models in that study were the Peng-Robinson (original and modified)[36,37], Soave-Redlich-Kwong[38,39], and

Benedict-Webb-Rubin equations of state[40]. It was found that the higher the boiling point of the cut, the less accurate the estimates were. Equation parameter adjustment by fitting to heavy compound properties did lead to improved simulation results. Heat capacity prediction of ill-defined hydrocarbons, using thermodynamic models is often challenging, since critical properties, mean molar mass and reference heat capacity values (ideal gas state) are unavailable. Thus, estimated liquid and gas heat capacity data from these methods are often inaccurate. Table 2.2 shows the range of data required for some the most popular prediction techniques of liquid isobaric heat capacity. Dadgostar and Shaw's innovative work showed again that the similarity concept allowed for reliable and accurate isobaric heat capacity predictions for ill-defined hydrocarbons[9,41]. Therefore, the similarity variable can be used as a prime basis for correlation development and extension, with fluid elemental analysis being its only input.

Table 2.2. Estimation Methods for Isobaric Liquid Heat capacity.

Estimation Method	Data Required	Method	Compound Range
Chueh-Swanson[26]	Molecular structure	GCM	Pure compounds
Missenerad[28]	Molecular structure	GCM	Pure compounds
Lee-Kesler[30]	T_c, P_c, ω	CSM	Pure compounds and mixture
Rowlinson – Bondi[31,32]	T_c, P_c, ω	CSM	Pure compounds and mixture
Reid Sobel / Tyagi[33]	Reduced Properties	TCM	Pure compounds
Dadgostar-Shaw[9]	Elemental Analysis	Similarity Variable	Wide range of HC, high MW HC, ill-defined mixtures

2.2 Similarity variable concept

The similarity variable, α, is rooted in quantum mechanics. It is a measure of the number of vibration modes per unit mass of a molecule or mixture that contribute to heat capacity. Molecular energy modes arise from translation, rotation, vibration and electronic excitation. Accordingly, the molar heat capacity of ideal gasses can be expressed as a function of three parameters (Equation 2-2) when internal vibration and electronic excitations are neglected.

$$\boldsymbol{C_p^{g0} = R + C_V^{translation} + C_V^{rotation} + C_V^{vibration}} \tag{2-2}$$

This can be further expressed in a simple RRHO model for linear molecule as the following:

$$\boldsymbol{C_V^{translation} = {}^{3}/_{2}\, R} \tag{2-3}$$

$$\boldsymbol{C_V^{rotation} = R} \tag{2-4}$$

$$C_{p,linear}^{g0} = R + {}^{3}/_{2}\, R + R + R \sum_{i=1}^{3N-5} \frac{\left(\frac{h\vartheta_i}{k_B T}\right)^2 - \exp\left(\frac{h\vartheta_i}{k_B T}\right)}{[1 - \exp\left(\frac{h\vartheta_i}{k_B T}\right)]^2} \tag{2-5}$$

And for non-linear molecules as the following:

$$\boldsymbol{C_V^{translation} = {}^{3}/_{2}\, R}$$

$$\boldsymbol{C_V^{rotation} = {}^{3}/_{2}\, R} \qquad (2\text{-}6)$$

$$C_{p,nonlinear}^{g0} = R + {}^{3}/_{2}\, R + R + R \sum_{i=1}^{3N-5} \frac{\left(\frac{h\vartheta_i}{k_B T}\right)^2 - \exp\left(\frac{h\vartheta_i}{k_B T}\right)}{[1 - \exp\left(\frac{h\vartheta_i}{k_B T}\right)]^2} \qquad (2\text{-}7)$$

Where,

$C_V^{translation}$*: Contribution to the molar heat capacity at constant volume from the translational motion of a molecule as a whole/* $J{\cdot}K^{-1}{\cdot}mol^{-1}$

$C_V^{rotation}$*: Contribution to the molar heat capacity at constant volume from the rotational motion of a molecule as a whole/* $J{\cdot}K^{-1}{\cdot}mol^{-1}$

$C_V^{vibration}$*: Contribution to the molar heat capacity at constant volume from the intramolecular vibrations in a molecule,* $J{\cdot}K^{-1}{\cdot}mol^{-1}$

T: is the temperature / Kelvin

R: is the universal gas constant/ $J.K^{-1}.mol^{-1}$

ϑ_i*: are the frequencies of vibrations of the* i^{th} *normal mode / Hz*

k_B*: is the Boltzmann constant/* $J.K^{-1}$

h*: is the Planck constant/ J.s*

As temperatures decrease to zero Kelvin, the individual contributions of the vibration mode approach zero. Whereas, at high temperatures, internal vibration mode

contributions to the ideal heat capacity increase and dominate the fewer and saturated rotation and translation modes. An example of molar heat capacities is shown below in Figure 2.1a. As expected, the ideal gas isobaric heat capacity increases with molar mass (at fixed temperature) and with temperature (fixed molar mass). However, Laštovka and Shaw[4] demonstrated that mass based ideal gas heat capacity was not primarily dependent on molecular size or structure or elemental composition, as shown in Figure 2.1b. for the same compounds. All three molecules share the same number of vibrations per mass since they have the same elemental composition (C_nH_{2n}), while they are different molecule sizes and structures. Even so, their specific heat capacities are almost identical. Accordingly, when dealing with molecules with high molar mass, the ideal gas heat capacity becomes primarily a function of the number of vibrations per unit mass, regardless of the specific nature of these internal vibrations. Laštovka's work lead to the proposition of the similarity variable concept that is a function of the elemental composition of a certain compound or mixture.

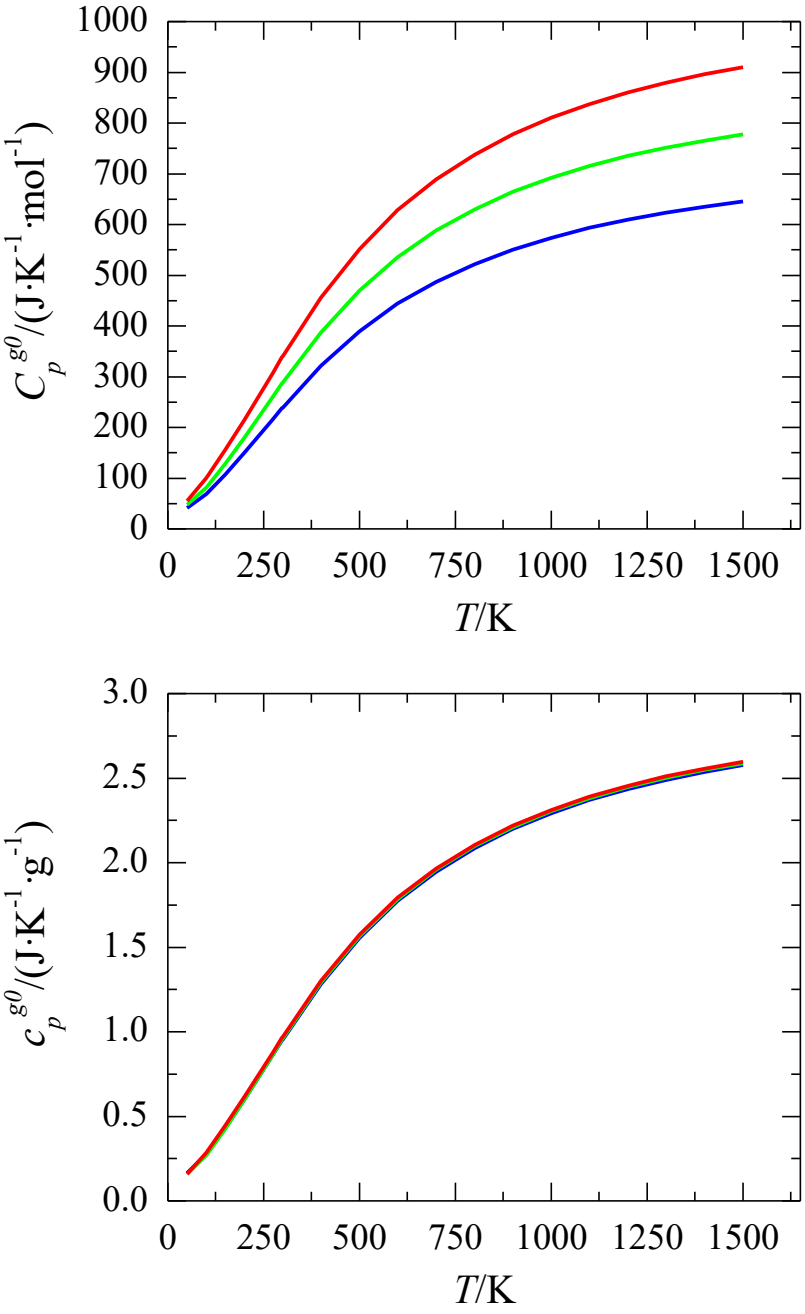


Figure 2.1: Thermodynamic Research Center (TRC)[42] recommended molar (a) and specific (b) heat capacity for large aromatic compounds originating from QM calculations. ——, Dicyclopenta[cd,fg]pyrene ($C_{20}H_{10}$, M=250.3 g·mol^{-1}, 84 vibration modes); ——, coronene ($C_{24}H_{12}$, M=300.6 g·mol^{-1}, 102 vibration modes); ——, Phenanthro[1,10,9,8-opqra]perylene ($C_{28}H_{14}$, M= 350.4 g·mol^{-1}, 120 vibration modes)[4]

The number of vibration modes, (f), per unit mass, (m), is related to the number of atoms in a large molecule (N) per unit mass following Eq. (2-8):

$$\varphi = \frac{f}{m} \cong \frac{N_A 3N}{M} = \frac{3N}{m} \tag{2-8}$$

Equation (2-8) can be determined from a mass composition based elemental analysis. Accordingly, the similarity variable alpha is further defined as:

$$\alpha = \frac{N}{M} = \frac{\sum_{i=1}^{n} v_i}{\sum_{i=1}^{n} v_i M_i} = \frac{\sum_{i=1}^{n} x_i}{\sum_{i=1}^{n} x_i M_i} = \frac{\sum_{i=1}^{n} \frac{w_i}{M_i}}{\sum_{i=1}^{n} w_i} \tag{2-9}$$

Where,

m:is the unit mass/ g

n: is the number of elements in a compound

N: is the number of atoms in a compound

M: is the molar mass of the compound/ g.mol^{-1}

M_i:is the molar mass of chemical element i/ g.mol^{-1}

x_i: is the mole fraction of element i in a compound/ mol

w_i: is the mass fraction of element i/ g

v_i: is the stoichiometric coefficient for element i in a compound

The literature focuses on the properties of small molecules both from a measurement and a prediction perspective. Thus, it focuses on impacts related to whole molecules which are more variable and structure specific. For larger molecules, atomic vibration effects dominate and if the differences atomistic vibrations are ignored (T_{sat},

frequency), the specific heat capacity becomes a function of the number of atoms in a molecule divided by its molar mass. The robustness and validity of this similarity variable and correlations making use of it for predicting constant specific heat capacities pure and ill-defined compounds for ideal gases, organic solids and liquids have been demonstrated by Dadgostar-Shaw[9,41] and Laštovka-Shaw[7,10,43].

Nevertheless, deviations from the similarity variable are also expected for certain families of compounds. In Figure 2.2 we can see ideal gas isobaric heat capacity trends for four molecules with the same similarity variable value. When dealing with acyclic linear hydrocarbons (solid lines), 1-undecene and 1-octadecene showed confounding heat capacity trends in accordance with the similarity variable concept. The same can be said about cyclic hydrocarbons (dashed lines), 1,1 dimethylcyclohexadecane compared to 1,1,4,4 tetramethylcyclohexadecane. However, a change of slope in the c_p^{g0} curve was observed[4] when comparing these two sets of compounds. This suggests that for high-precision heat capacity estimation, universal coefficients for the predictive correlations should be derived specific to families of compounds.

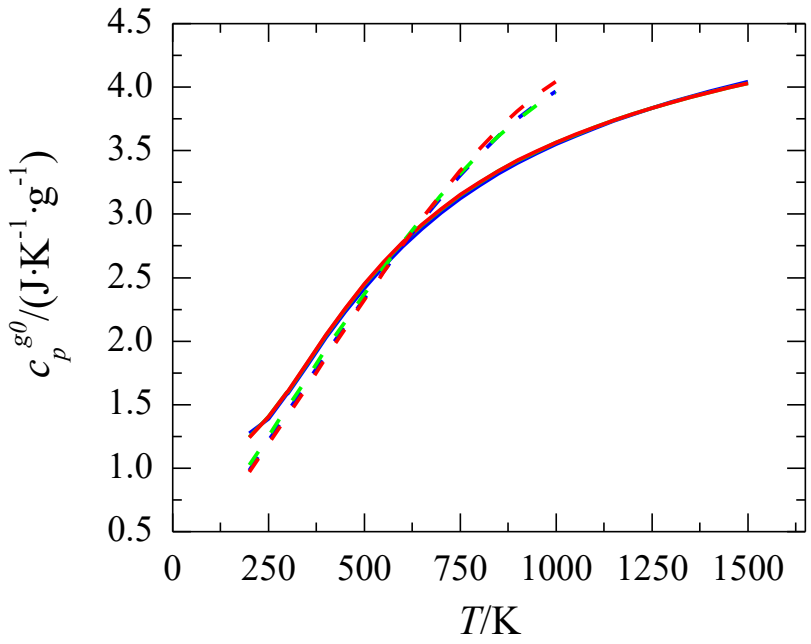


Figure 2.2: TRC recommended specific ideal gas heat capacity data for aliphatic hydrocarbons with similar α [4] Solid lines – acyclic linear unsaturated hydrocarbons: —— blue line, 1-undecene ($C_{11}H_{22}$, M=154.3 g·mol^{-1}) —— green line, 1-octadecene ($C_{18}H_{36}$, M=252.5 g·mol^{-1}); —— red line, 1-eicosene ($C_{20}H_{40}$, M=280.5 g·mol^{-1}) **Dashed lines –** cyclic saturated hydrocarbons [24]: - - - blue dotted line, 1,1-dimethylcyclohexadecane ($C_{18}H_{36}$, M=252.5 g·mol^{-1}); - - - green dotted line 1,1,4,4-tetramethylcyclohexadecane ($C_{20}H_{40}$, M=280.5 g·mol^{-1}); - - - red dotted line cyclooctacosane ($C_{28}H_{56}$, M=392.7 g·mol^{-1})

As for heteroatom containing molecules, increased variation in heat capacity prediction is related to the heteroatom's type, functional group and mass fraction. In the case of N-methylcarbazole (7.7 wt.% N) and 1-pentylcoronene, deviation in computed values were found to be at 6.7% (Figure 2.3). However, in the case N,N'-diphenylcarbodiimide (14.4 wt.% N) and fluoranthene, high deviation in computed was value observed below 600K, with an average relative deviation of 9% over the whole temperature range (Figure 2.4).

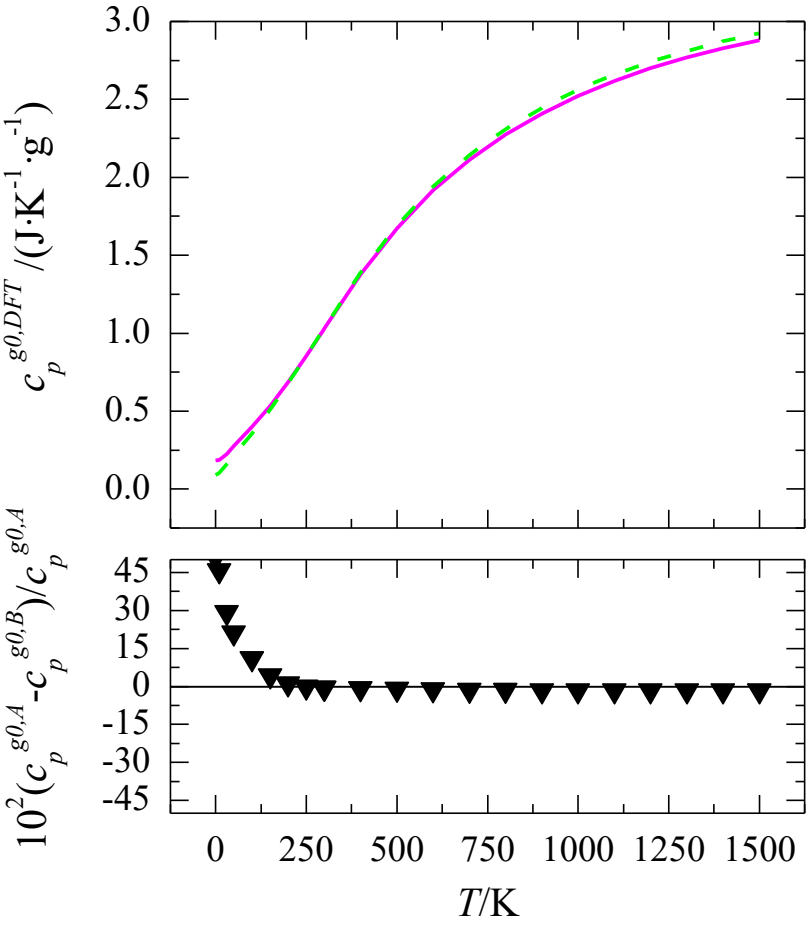


Figure 2.3:DFT RRHO computed temperature dependences of c_p^{g0} for[4]: —— magenta line, N methylcarbazole (C13H11N; M=181.2 g·mol 1, ∝ = 0.1379 mol·g 1); - - - green dotted line, 1 pentylcoronene (C29H22, M=370.5 g·mol 1, ∝= 0.1377 mol·g 1). Lower insert: relative deviation of the computed $c_p^{g0,DFT}$ values of *N*-methylcarbazole (A) from 1-pentylcoronene (B).

Heteroatom containing functional groups have significantly different IR absorption wavenumbers, as well as different skeletal vibration modes. Thus, this will lead to a deviation in heat capacity of the associated compounds. Still, Laštovka[4] argued that at low heteroatom mass fraction these differences fall within acceptable prediction errors. Accordingly, the similarity variable concept is recommended for applications where heteroatom content falls below 15 wt.%.

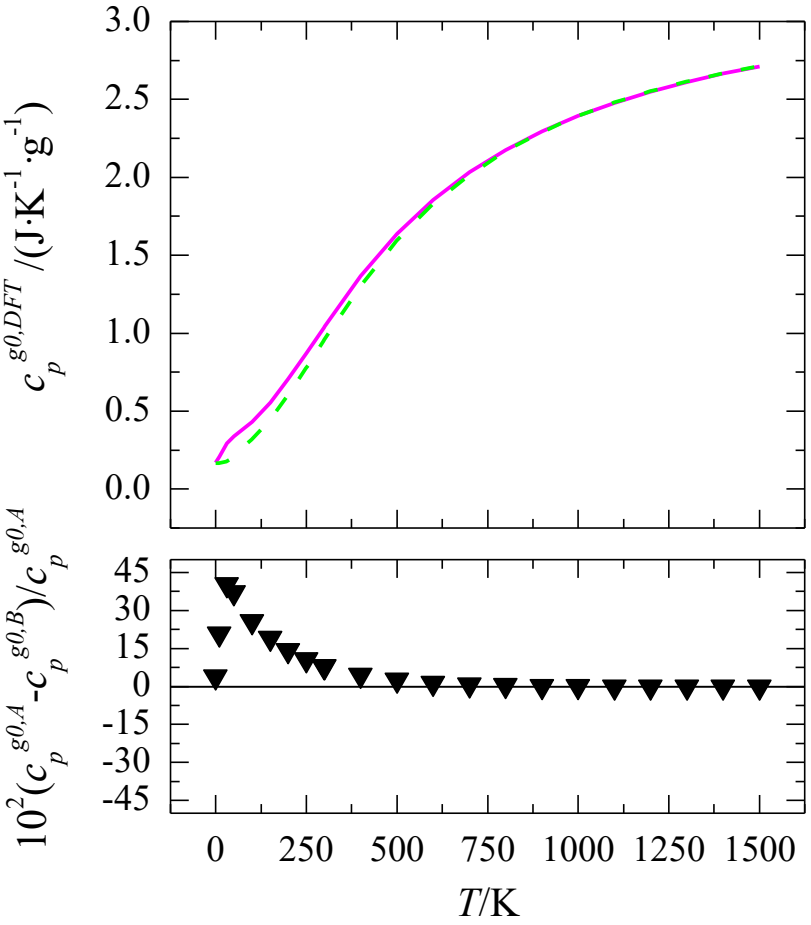


Figure 2.4: DFT RRHO computed temperature dependences of c_p^{g0} for[4]: —— magenta line, N,N' diphenylcarbodiimide (C13H10N2, M=194.2 g·mol 1, α = 0.1287 mol·g 1); - - - green dotted line, fluoranthene (C16H10, M= 202.3 g·mol 1, α = 0.1286 mol·g 1). Lower insert: relative deviation of the computed $c_p^{g0,DFT}$ values of *N*,*N*'-diphenylcarbodiimide (A) from fluoranthene (B).

These results suggest there might be potential in introducing a correction factor based on mass fraction of heteroatom to the predictive correlations, if the similarity variable concept was to be extended to >15 wt.%

2.3 Thesis objectives

The principal objective of the thesis is to extend the range of application of the liquid and solid heat capacity (c_p) correlations, that are based on the similarity concept, to include high heteroatom content compounds from biodiesels to sugars. Specific tasks are to:

- Develop more accurate fluid family specific c_p correlations by reparametrizing the current hydrocarbon only correlations.
- Detect trends of the secondary (atom type) and tertiary (structure) effects using data from the heat capacity database.
- Collect heat capacity data of some sugars using differential scanning calorimetry (DSC), to test the specific solid heat capacity (c_{pLS}) correlation on highly oxygenated compounds.
- Collect biodiesel heat capacity data from the literature, to test the specific liquid heat capacity (c_{pDS}) correlation performance for highly oxygenated compounds.
- Introduce an adjustment parameter to encompass secondary effects and produce high accuracy correlations for both solids and liquids

3 Developing Family Specific Heat Capacity Correlations for Solid and Liquid Hydrocarbons

3.1 Introduction

Following on from the success with developing predictive correlations based on the robust similarity variable concept, the goals of this work are to create high-precision predictive correlations for individual compounds, specific mixed fluids, and chemical families of solid and liquid compounds, without the introduction of functional-group specific parameters. First, the parameterization of the correlations is reviewed to ensure the correlations are optimized with respect to temperature and values of the similarity variable (α) for the existing database. Second, optimum sets of parameters for chemical families within the database are explored. The main application of family specific correlations would be to provide more precise characterization of key compound classes used commonly in industry. Findings arising from these preliminary investigations informed exploration on how to optimize correlations for specific families of compounds and mixtures by introducing tailored parameters based on family specific attributes.

3.2 Solid heat capacity correlation

Laštovka et al.[8], developed a predictive correlation for specific heat capacity (c_{pLS}) of organic solids, based on the similarity variable concept. The correlation (equation 3- 1) has a wide range of applications; valid from 50K to the fusion temperature of the

respective compound. Applications include c_{pLS} estimation for pure organic solids, ill-defined solid organic mixtures, and provision of a baseline for detecting phase changes in ill-defined hydrocarbon fractions.

$$c_{pLS} = 3(A_1\alpha + A_2\alpha^2)R\left(\frac{\theta}{T}\right)^2 \frac{exp\left(\frac{\theta}{T}\right)}{\left[exp\left(\frac{\theta}{T}\right) - 1\right]^2} + (B_1\alpha + B_2\alpha^2)T + (C_1\alpha + C_2\alpha^2)T^2$$

(3-1)

Equation 3-1 includes two variables, temperature (T) and α, and seven universal coefficients. The above correlation was developed by introducing the similarity variable concept and re-parameterizing the Briard et al.[22] four-parameter equation for the molar heat capacity for n-alkanes:

$$C_p^s = 3AR\left(\frac{\theta}{T}\right)^2 \frac{exp\left(\frac{\theta}{T}\right)}{\left[exp\left(\frac{\theta}{T}\right) - 1\right]^2} + bT + cT^2$$

(3- 2)

In equation 3-2, the parameters *A, θ, b* and *c* are functions of the number of carbons in the alkane chain, and *R* is the ideal gas constant. These parameters are expressed as power series of second order as functions of the similarity variable alpha (α), in equation 3-1. The first term in equation 3-1 is a modified Einstein term, which accounts for molecular vibrations saturating at low temperatures. The database[4] of compounds used to derive the correlations consisted of 165 compounds ranging over 9 chemical families: Alkanes, Alkenes, Alcohols, Aromatic, Carboxylic Acids, Esters, Naphthene, SNO containing compounds, and Triglycerides. The database consisted of

4100 data points, where the temperature spanned from 50K to melting and the molar mass spanned from 130.2 to 1100 g.mol^{-1}. The database was divided into a training set of 72 compounds (2020 data points) and a test set of 93 compounds (2080 data points). The universal parameters were then regressed from the training set and the goodness of fit of the correlation was calculated using the test set. The performance of equation 3-1 was found to be great, with an average absolute deviation for the test data set of 0.068 J K^{-1} g^{-1}.

3.3 Liquid heat capacity correlation

Dadgostar and Shaw devised a correlation for organic liquids including pure organic compounds as well as Ill-defined mixtures like bitumen and heavy oil[9,41]. The similarity variable was introduced this time to the widely-used Lee-Kesler correlation[30] that relates heat capacity to temperature and specific gravity:

$$C_p^l = A_1 + A_2 T + A_3 T^2$$

$$A_1 = -1.171126 + (0.023722 + 0.024907 spgr) K_w + \frac{1.14982 - 0.046535 K_w}{spgr}$$

$$A_2 = (10^{-4})(1.0 + 0.82463 K_w)\left(1.12172 - \frac{0.27634}{spgr}\right)$$

$$A_3 = (10^{-8})(1.0 + 0.82463 K_w)\left(2.9027 - \frac{0.70958}{spgr}\right)$$

(3- 3)

where,

C_p^l: is the isobaric heat capacity of liquid petroleum fraction in / Btu.lb^{-1}. degree Rankine^{-1}

K_w: is the Watson characterization factor

spgr: is the specific gravity/ 60 F

valid from approximately 0.4 < Tr ≤ 0.85 / reduced temperature degree Rankine

With the introduction of the similarity concept, equation 3-3 becomes:

$$c_{pDS} = a_1 + (a_{21}\alpha + a_{22}\alpha^2)T + (a_{31}\alpha + a_{32}\alpha^2)T^2$$

$$a_1 = (a_{11}\alpha + a_{12}\alpha^2) \times 3R\left(\frac{\theta}{T}\right)^2 \frac{\exp(\theta/T)}{[\exp(\theta/T) - 1]^2}$$

$$T > 200K$$

$$a_1 = (a_{11}\alpha + a_{12}\alpha^2) \times 24.5$$

(3- 4)

Equation 3-4 includes the similarity variable (α) and temperature as second order power series and six universal coefficients. When temperature is higher than 200K the first term of the equation (a_1) is reduced to a function of the similarity variable only. The database[41] of compounds used to derive the correlations consisted of 37 compounds ranging over five chemical families: Alkanes, Aromatic, Naphthene, SNO containing compounds, and Molten Polymers. The database consisted of 261 data points, where the temperature spanned from 196K to 620K and the molar mass

spanned from 100.2 to 290.53 $g.mol^{-1}$. The database was divided into a training set of 22 compounds (150 data points) and a test set of 15 compounds (111 data points). The universal parameters were then regressed from the training set and the goodness of fit of the correlation was calculated using the test set. The performance of equation 3-1 was found to be great, with an average absolute deviation for the test data set of 0.035 $J. K^{-1}. g^{-1}$

Equation 3-4 is preferred over the original Lee-Kesler equation based on its greater accuracy and its broader range of application. Comparison between the Lee-Kesler correlation and Dadgostar-Shaw correlation showed a decrease in prediction average relative error from 5% to 3.2% for the same dataset[41]. Equation 3-4 was modified recently to provide better agreement near liquid-vapour critical points as well[9].

3.4 Functional Form optimization

Constant pressure heat capacity correlations are usually power series in temperature. It is important to find optimal functional forms linking databases and characteristic variables as part of correlation generation and optimization processes. Both the Dadgostar-Shaw and Laštovka -Shaw correlations were based on well established second order polynomial correlations. In this work, function optimization was examined for temperature and the similarity variable to rule out other possible options for parametrization, and to confirm the choice of models made for the database (Lee-Kesler and Briard).

3.4.1 Methodology and Databases

The same constant pressure heat capacity databases that were used to regress universal coefficients for the Dadgostar-Shaw and Laštovka -Shaw correlations were used in this work. The solid database included data for 165 organic compounds from different chemical families culled from the literature. Most of the data was smoothed based on comprehensive analysis, with uncertainty within the confines of experimental error. Detailed sources of the database can be found, in recent published work[8]. For the fitting of the seven universal coefficients the database was divided into a training set and a test set. The training set comprised 72 organic compounds. For the purpose of this work the compounds were divided into their chemical families: alkanes, alkenes, alcohols, esters, carboxylic acids, naphthenes, aromatics, heteroatom containing compounds and triglycerides. The detailed database can be found in Appendix A.

The liquid constant pressure heat capacity database comprises unsmoothed, experimental liquid heat capacity data for 31 organic compounds and six molten polymers carefully selected from the literature to have minimal uncertainties. The detailed sources of the liquid database can be found in a previously published work[41]. The molar masses in the database range from 100.2 to 290.53 $g.mol^{-1}$ for the 31 organic compounds in the temperature range from 196 to 560 K. For the polymers, the temperature range was from 347.61 to 620 K. To fit the six universal parameters in the correlation, the database was divided into a training set and a test set. The training set included 19 organic compounds from various chemical families and three molten polymers. The test set, comprised 12 organic compounds and three molten polymers. For this work, the liquid constant pressure heat capacity database was divided into the constituent chemical families: alkanes, naphthenes, aromatics, and heteroatom containing compounds. The detailed database can be found in Appendix B.

3.4.2 Functional Form Optimization for Solids

In Laštovka's work, no alternate functional forms as a function of temperature (T) and similarity variable (α) were explored. Based on the work done by Sallamie and Shaw[45], the Einstein term was simply introduced to the well established second order power series numerical model developed by Briard et al.[22] (Equation 3-2). The similarity variable was also introduced as a second order polynomial. In this work we explored other polynomial relationships between heat capacity (c_{pLS}) and the

variables, Temperature (T), and similarity variable (α). Four polynomials were explored:

(1) $c_{pLS} = a + bT + cT^2$

(2) $c_{pLS} = a + bT^{1/2} + cT$

(3) $c_{pLS} = a + bT + cT^{-1}$

(4) $c_{pLS} = a + bT^{-1} + cT^{-2}$

(3- 5)

The database was divided into chemical families; then for each compound c_{pLS} vs T was regressed and plotted for all four polynomials. Parameters for the correlations were found using the Ordinary Least Square method (OLS), by minimizing the objective function *S*:

$$S = \sum_{i=1}^{m} \sum_{j=1}^{n} \left(c_p^{exp} - c_p^{cal}\right)^2 / n$$

(3- 6)

where,

c_p^{exp}*: experimental value of heat capacity/ J.K*$^{-1}$*.g*$^{-1}$

c_p^{cal}*: calculated value of heat capacity/ J.K*$^{-1}$*.g*$^{-1}$

n: number of experimental data

m: number of compounds

All regression work was done using the curve fitting tool in MATLAB, where the quality of iterations is reported as a sum of square error (SSE):

$$SSE = \frac{\sum_{i=1}^{n}\left(c_p^{exp} - c_p^{cal}\right)^2}{n} \tag{3- 7}$$

and as a root mean square error (RMSE):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}\left(c_p^{exp} - c_p^{cal}\right)^2}{n}} \tag{3- 8}$$

SSE and RMSE were used iteratively to identify the best functional form for individual compounds and then for chemical families.

An example illustrating the goodness of fit of the four polynomials at the family level is shown in Table 3.1 for Alcohols. It is evident that the best functional form is a second order polynomial in temperature i.e. Equation 3-5 (1). This result was expected, given the success of the Briard correlation.

Table 3.1: Goodness of fit of the four polynomials (1), (2), (3), and (4) for Alcohols

	Equation 3-5 (1)	**Equation 3-5 (2)**	**Equation 3-5 (3)**	**Equation 3-5 (4)**
SSE	2.9 E-02	5.2 E-02	4.1 E-02	1.5 E-01
RMSE	2.3 E-02	3.1 E-02	3.3 E-02	5.2 E-02

Secondly, the functionality relative to the similarity variable, α, was explored. Each of the coefficients A, B and C of the general c_{pLS} correlation (Equation 3-1) was calculated and then regressed versus the similarity variable, α. This work was also conducted using the curve fitting tool on MATLAB. A secondary polynomial relationship as a function of the similarity variable was observed in most cases, suggesting that the original form introduced to the Briard correlation was the best choice.

3.4.3 Functional Form Optimization for Liquids

The first step in finding the best functional form for the liquid isobaric heat capacity correlation was to find the best relationship between heat capacity (c_{pDS}) and the variable, Temperature (T). According to the review done by Zabransky and Růžička[2], most liquid heat capacity prediction correlations are a function of a second order temperature polynomial, nonetheless there could be some exceptions, like in the case of alcohols where a first order polynomial was recommended. Accordingly, other functionalities in terms of temperature are plausible. Four polynomials were explored in this work, for temperatures remote from critical point:

(1) $c_{pDS} = a + bT + cT^2$

(2) $c_{pDS} = a + bT^{1/2} + cT$

(3) $c_{pDS} = a + bT + cT^{-1}$

(4) $c_{pDS} = a + bT^{-1} + cT^{-2}$

(3- 9)

An example illustrating the fitting process at the compound level is shown in Figure 3.1 for Xylene (C_8H_{10}). The goodness of fit criteria for xylene using the four proposed polynomials are shown in Table 3.2. It is evident that the best functional form is a second order polynomial in temperature i.e. Equation 3-9 (1). This result was expected, given the success of the Lee-Kesler correlation.

Table 3.2: Goodness of fit of the four polynomials (1), (2),(3), and (4) for C_8H_{10} (aromatic)

	Equation 3-9 (1)	**Equation 3-9 (2)**	**Equation 3-9 (3)**	**Equation 3-9 (4)**
SSE	7.4 E-08	4.15 E-05	1.15E-07	1.36 E-07
RMSE	1.9 E-04	4.5 E-03	2.4 E-04	2.6 E-04

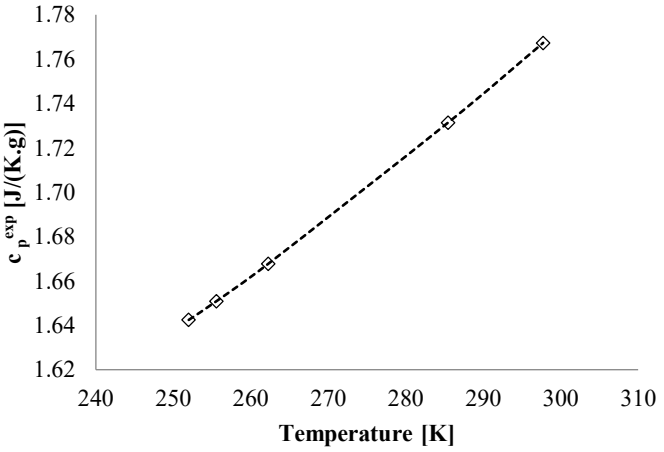


Figure 3. 1:-♦-♦- Experimental heat capacity distribution versus temperature of C8H10 (Aromatic)

The second step was to explore the functionality relative to the second variable, α. Each of the coefficients a_1, a_2 and a_3 of the general c_{pDS} correlation (Equation 3-3) was calculated and then regressed versus the similarity variable, α. This work was also conducted using the curve fitting tool on MATLAB. Results were explored relative to the different chemical families, except for aromatics, due to the small number of data.

An example illustrating the fitting process for the paraffin family is presented in Figure 3.2.

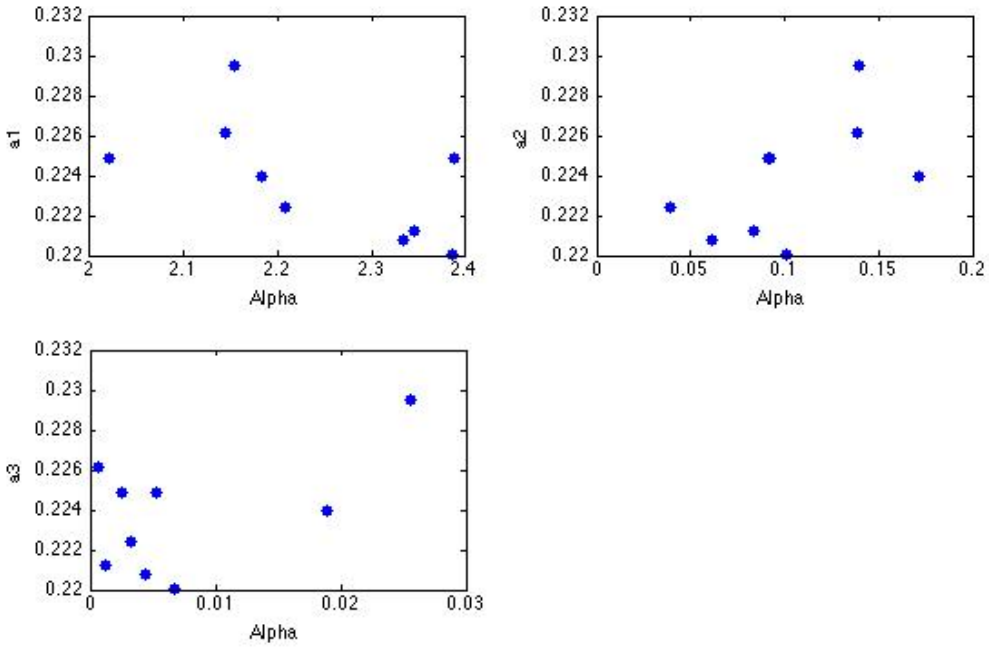


Figure 3.2:a1, a2, and a3 versus alpha for the liquid Alkane family

No clear or prominent trends were observed for the different data sets. Accordingly, no functional form changes are suggested for the Dadgostar-Shaw correlation.

3.5 Developing Chemical Family Specific Forms

3.5.1 Method

The goal of this work was to produce family specific heat capacity correlations, by adjusting one or two of the existing coefficients while retaining the overall reliability of the functional form. Focus was put primarily on adjustments to the first term in equations 3-1 (A_1, A_2, θ) and 3-4 (a_{11}, a_{22}) which are common to liquids and solids. The coefficients were varied within an interval of -100% to +100% of their original values at 1% increments. All calculations were carried out using a customized MATLAB script that can be found in Appendix C. Outcomes from Laštovka-Shaw (LS) and Dadgostar-Shaw (DS) were compared with the data generated by the adjusted correlations (New) in tables 3.3. and 3.4., respectively.

3.5.2 Results

3.5.2.1 Solid families

Adjustment to A_1, A_2, and θ reduced the absolute average error for some of the families of compounds. For alkanes, deviations were already below 2% and parameter adjustment had little effect. For other families, their parameter adjustment reduced the percent deviations. The family specific parameters are shown in Table 3.2. and their impact on absolute deviation (Equation 3-10) and absolute relative deviation (Equation 3-11) are summarized in Table 3.3. For some families of compounds, the deviations remained large suggesting the need for an alternate optimization approach.

$$\delta = \frac{1}{m}\sum_{i=1}^{m}\left[\sum_{j}^{n}\sqrt{(c_p^{exp} - c_p^{calc})^2}_{j} \Big/ n\right]$$

(3-10)

$$\varepsilon = \frac{1}{m}\sum_{i=1}^{m}\left[\sum_{j}^{n}\sqrt{\left((c_p^{exp} - c_p^{calc}) \Big/ c_p^{exp}\right)^2}_{j} \Big/ n\right]$$

(3-11)

Table 3.3.: Adjusted coefficients for the solid isobaric heat capacity correlation (Equation 3-1)

	Family Specific Parameters								*Generalized Parameters*
		Alkanes	***Alkenes***	***Alcohols***	***Esters***	***Carboxylic Acids***	***Naphthenes***	***Aromatic***	***All Solid Families***
New Parameters	A_1	0.0119	0.0136	0.0141	0.0158	0.0142	0.0264	0.0264	0.013183
	A_2	0.2544	0.2993	0.2269	0.2993	0.2743	0.1421	0.0499	0.249381
	θ	151.8675	151.8675	151.8675	151.8675	151.8675	151.8675	151.8675	151.8675
	B_1	0.0265	0.0265	0.0265	0.0265	0.0265	0.0265	0.0265	0.0265
	B_2	-0.0249	-0.0249	-0.0249	-0.0249	-0.0249	-0.0249	-0.0249	-0.0249
	C_1	2.5096 E-05	2.5096 E-05	2.5096 E-05	2.5096 E-05	2.5096 E-05	2.5096 E-05	2.5096 E-05	2.5096 E-05
	C_2	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04	-1.23255 E-04
% Change	A_1	-10%	+3%	-7%	-20%	-8%	-100%	-100%	0
	A_2	+2%	+20%	+9%	-20%	-10%	+43%	+80%	0
	θ	0	0	0	0	0	0	0	0

Table 3.4.: Goodness of fit for the solid heat capacity correlation Equation 3-1 (LS) compared to the adjusted correlation (New) using the coefficients from table 3.3.

		Alkanes		*Alkenes*		*Alcohols*		*Esters*		*Carboxylic Acids*		*Naphthene*		*Aromatic*	
		LS	**New**	**LS**	**New**	**LS**	**New**	**LS**	**New**	**LS**	**New**	**LS**	**New**	**LS**	**New**
Training set	**δ**	0.01	0.01	0.05	0.01	0.02	0.01	0.11	0.05	0.03	0.02	0.06	0.05	0.08	0.06
	100. ε	1.56	1.55	5.46	1.66	2.37	1.57	9.51	4.66	2.77	1.62	7.88	6.64	10.5	7.71
Test set	**δ**	0.04	0.04	0.09	0.04	0.03	0.04	0.07	0.03	0.09	0.07	0.12	14.9	0.04	0.04
	100. ε	4.27	4.27	9.67	4.21	3.26	3.66	8.13	3.94	8.34	6.49	14.88	11.84	6.43	6.33

3.5.2.2 Liquid families

For liquids, adjustment to a_{11} and a_{12} reduced the absolute average error for some of the families of compounds (alkanes and naphtenes). For molten polymers, changing the parameters within 10% yielded a better performance for the training set but not for the test set. Hence, it is recommended to continue using the original parameters. The family specific parameters are shown in Table 3.5. and their impact on absolute and percent deviation are summarized in Table 3.6. For some families of compounds (aromatic and unsaturated cyclics), the deviations remained large even after attempting to adjust all six parameters. Accordingly, these results reiterate the need to explore another optimization approach for some of the liquid compounds.

Table 3.5: Adjusted coefficients for the liquid isobaric heat capacity correlation (Equation 3-4)

	Family Specific Parameters						*Generalized Parameters*
		Alkanes	***Naphthenes***	***Aromatics and Unsaturated cyclic***	***Compounds with heteroatoms (SNO)***	***Molten Polymers***	***All Liquid Families***
New Parameters	a_{11}	-0.3075	-0.3143	-0.5124	-0.3587	-0.3758	-0.3416
	a_{12}	2.1537	2.0404	3.2646	2.4938	2.4258	2.2671
	b_{11}	0.1064	0.1064	0.1064	0.1064	0.1064	0.1064
	b_{12}	-0.3874	-0.3874	-0.3874	-0.3874	-0.3874	-0.3874
	c_{11}	-9.8231 E-05	-9.8231 E-05	-9.8231 E-05	-9.8231 E-05	-9.8231 E-05	-9.8231 E-05
	c_{12}	4.18200 E-04	4.18200 E-04	4.18200 E-04	4.18200 E-04	4.18200 E-04	4.18200 E-04
% Change	a_{11}	-10%	-8%	+50%	-5%	-10%	0
	a_{12}	-5%	-10%	+44%	-10%	-7%	0

Table 3.6: Goodness of fit for the liquid heat capacity correlation Equation 3-4 (DS) compared to the adjusted correlation (New) using the coefficients from table 3.5.

		Alkanes		*Naphthenes*		*Aromatics and Unsaturated cyclic*		*Compounds with heteroatoms (SNO)*		*Molten Polymers*	
		DS	**New**	**DS**	**New**	**DS**	**New**	**DS**	**New**	**DS**	**New**
Training set	**δ**	0.049	0.034	0.095	0.042	0.122	0.096	0.140	0.121	0.059	0.040
	100. ε	2.254	1.590	4.941	2.104	6.157	4.379	7.323	6.540	2.489	1.628
Test set	**δ**	0.090	0.043	0.061	0.050	0.080	0.063	0.051	0.090	0.041	0.055
	100. ε	4.017	1.955	3.091	2.525	4.641	3.757	2.966	4.697	1.577	2.214

3.6 Summary

By employing numerical optimization, high-precision, chemical family specific, correlations were generated in the cases of:

- Alkenes, Alcohols, Esters, and Carboxylic Acids – for the solid heat capacity correlation
- Alkanes, Naphthenes, Compounds with Heteroatoms (SNO), and Molten Polymers – for the liquid heat capacity correlation

For other cases, no improvement over the general equations, equation (3-1) and (3-4) is obtained and improvement must rely on incorporating additional and easily accessible information about a family of compounds: atom type attributes and structural attributes. In this way, the limits of the similarity variable concept are overcome and isobaric heat capacities for high heteroatom containing molecules, found in the biofuels, sugars and pharmaceutical industries can be accommodated.

4 Extending the Solid Isobaric Heat Capacity correlations to compounds with more than 15 wt. % Sulfur, Nitrogen and Oxygen combined

4.1 Introduction

When trying to develop high precision, family specific, isobaric heat capacity correlations, it was observed that for families of compounds with high aromatic or heteroatom content, the numerical optimization of the current functional form fails. To produce high accuracy correlations for these families, secondary atom type effects and tertiary molecular structure must be explored. Laštovka[4] had observed that a deviation from the similarity variable arises when dealing with a heteroatom content higher than15 wt.%., as well as a deviation in the shape of the c_p^{g0} slope for compounds that possess the same value of the similarity variable but different molecular structures (cyclic vs. acyclic aliphatic compounds). In order to expand the correlation to include families of specific interest, sugars and biofuels, the introduction of a parameter that addresses the deviation caused by oxygen, sulfur, nitrogen, and cyclic configurations is considered.

4.2 Measuring Solid Heat Capacity for Sugars Using Differential Scanning Calorimetry (DSC)

Sugars are some of the basic and most widely used ingredients in the food and pharmaceutical industries[46]. Sugar contributes many qualities to products from flavor, to texture, to increased shelf life. Moreover, it can also act as a carrier of the active component for many medications.

To ensure these product quality attributes, production processes must be optimized. Hence, sugar properties must be accurately characterized for use in specific applications. One of the most common methods used to characterize sugars is through their melting behaviour. Thermal analytical techniques, like Differential Scanning Calorimetry (DSC) may be used[46,47]. These methods are fast, and easy. When a sugar melts, an onset melting temperature (T_m onset), a peak melting temperature (T_m peak), and an enthalpy of fusion (ΔH) are obtained using DSC experiments. These parameters are subsequently used to identify and characterize sugars based on purity, type, and size[48]. However, many sugars undergo transitions from one solid crystal state to another, or to a liquid crystalline state prior to melting, and many sugars decompose rapidly in the liquid state[49] complicating the identification, analysis and attribution of "peaks" in calorimetric data. Consequently, reported melting temperatures/behaviours can vary widely for the same material. Other attributions for differences among values include: different determination methods, origin, impurity, polymorphs, and superheating. Melting parameters are not reliable for characterization, and therefore, alternative approaches to predict thermal behaviours of sugars are needed.

Solid-state isobaric heat capacities were measured for seven sugars using a Differential Scanning Calorimeter (DSC). The instrument was calibrated carefully before each experiment to ensure the highest reproducibility and accuracy for the data. Each experiment was reproduced three times. The experimental heat capacity for these sugars was then compared to predicted values using the Laštovka-Shaw predictive correlation (Equation 3-1) for solids and to the heteroatom adjusted predictive correlation (Equation 4-1).

4.2.1 Differential Scanning Calorimetry (DSC)

Differential Scanning Calorimetry (DSC) is one of the most widely used thermal analysis techniques[50]. In this work, the Heat Flux mode was used, where the signal measured is the difference in temperature between a sample and a control. Both steady state and non-steady state phenomena can occur in this type of measurement. Only apparent heat capacities of the sample and the reference cells are considered. Heat loss and inter cell interactions are neglected. Typically heat capacity and melting points are readily distinguished. DSC curves are also often used to identify un-known samples and their physical characteristics from phase diagrams to the degree of crystallinity[51-54]. The measurement was conducted on a Setaram TG-DSC 111. This device includes a CS 32 processing unit and an assembly coupling a B111 microbalance to the DSC 111 calorimeter as shown in Figure 4.3. A Schematic, Figure 4.4, illustrates the calorimetric block. Thermocouples that carry the heat-flux transducers, wrap around the central part of the alumina tubes where the sample and the control are located. The samples were contained in 100 mm^3 stainless-steel crucible, sealed with a stainless-steel lid and a nickel ring. The sealed crucible was pressure rated at 20 bar and the samples were run with flowing inert gas in the calorimetric chambers.

Figure 4. 1:TG-DSC 111 apparatus

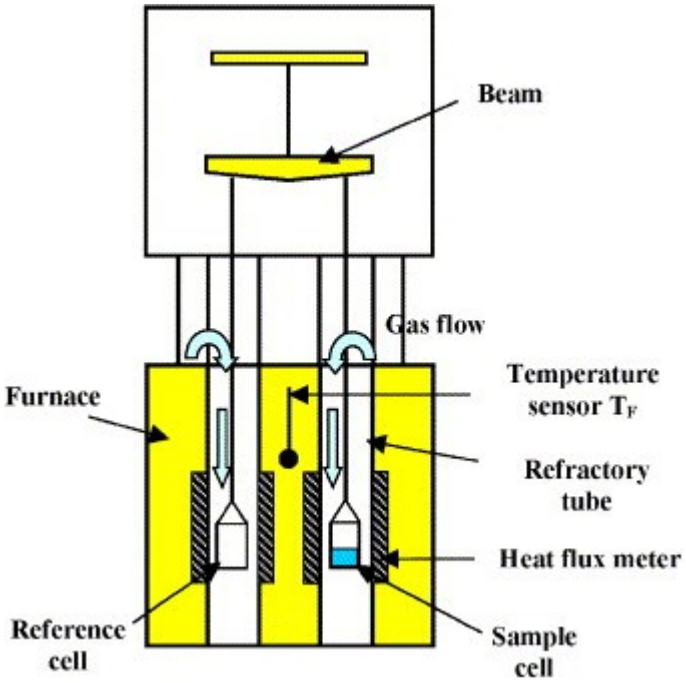


Figure 4. 2:Schematic of the cell setup in the TG-DSC 111 Setaram

4.2.1.1 Calibration

The calibration of the DSC was done following recommendations from the German Society of Thermal Analysis (GEFTA). Temperature calibration to ITS 90 was conducted using indium (NIST standard reference material 2232), tin (NIST SRM 2220), lead and aluminum. As for the energy calibration, they were carried out by measuring the heat of fusion of naphthalene, a reference material[55,56]. The energy measurement accuracy was within 2% compared to literature[57,58]. For the calibration of heat capacity, C_p, synthetic sapphire was used as primary reference and naphthalene was a secondary reference, as recommended by NIST (SRM 720). Experimental error in C_p measurements was less than

4% (0.05 J/(K·g)) in the temperature range of 210 K to 300 K (liquid nitrogen cooling was used) and less than 2 % (0.02 J/(K.g)) in the range of 300 K to 560 K.

4.2.1.2 Experimental Methodology

Every experiment included 4 steps, first the crucibles were run blank, then additional calibration was carried out using two different masses of synthetic sapphire (101.05 mg and 105.30 mg). The purpose of these calibrations was to ensure accuracy and reproducibility of measurements. The scanning rate was set to 5 ºC/min and the temperature range varied from 300 K to 573K depending on the melting points of the sugar sample to follow. After that the sugar sample was measured. The heat capacity of the samples was then calculated following the equations below:

$$c_{p,sample}(T) = \frac{HF_{sample} - HF_{blank}}{HF_{sapphire} - HF_{blank}} \times \frac{Mass_{sapphire}}{Mass_{sample}} \times c_{p,sapphire}(T) \quad (4\text{-}1)$$

Where,

HF_{blank} is the heat flow from run 1(empty crucibles)

$HF_{sapphire}$ is the heat flow from run 2

HF_{sample} is the heat flow from run 3

The value for $c_{p,sapphire}$ is obtained from the Archer Equation:

$$c_{p,sapphire} = aT^6 + bT^5 + cT^4 + dT^3 + eT^2 + fT + g \quad (4\text{-}2)$$

Coefficient values for equation 4-3 are listed in Tables 4.1. and 4.2.

Table 4.1: Coefficient for Archer equation at temperature higher than 20 C

Coefficient	Value
a	$1.197441280319*10^{-17}$
b	$-2.5923466515291*10^{-14}$
c	$1.3104884522373*10^{-11}$
d	$1.1963323706663*10^{-8}$
e	$-1.8121828407681*10^{-5}$
f	$9.2237456478216*10^{-3}$
g	-0.73178005598711

Table 4.2: Coefficient for Archer equation at temperature lowers than 20 C

Coefficient	Value
a	$1.82625552716194*10^{-15}$
b	$-3.20804888607333*10^{-12}$
c	$2.33660045792947*10^{-9}$
d	$-8.94387101696165*10^{-7}$
e	$1.8175474167972*10^{-4}$
f	-0.0144995136493316
g	0.457354829163823

Figure 4.5 shows the sapphire heat capacity calibration curve for two different experiments, compared to the sapphire heat capacity calculated from Archer's equation.

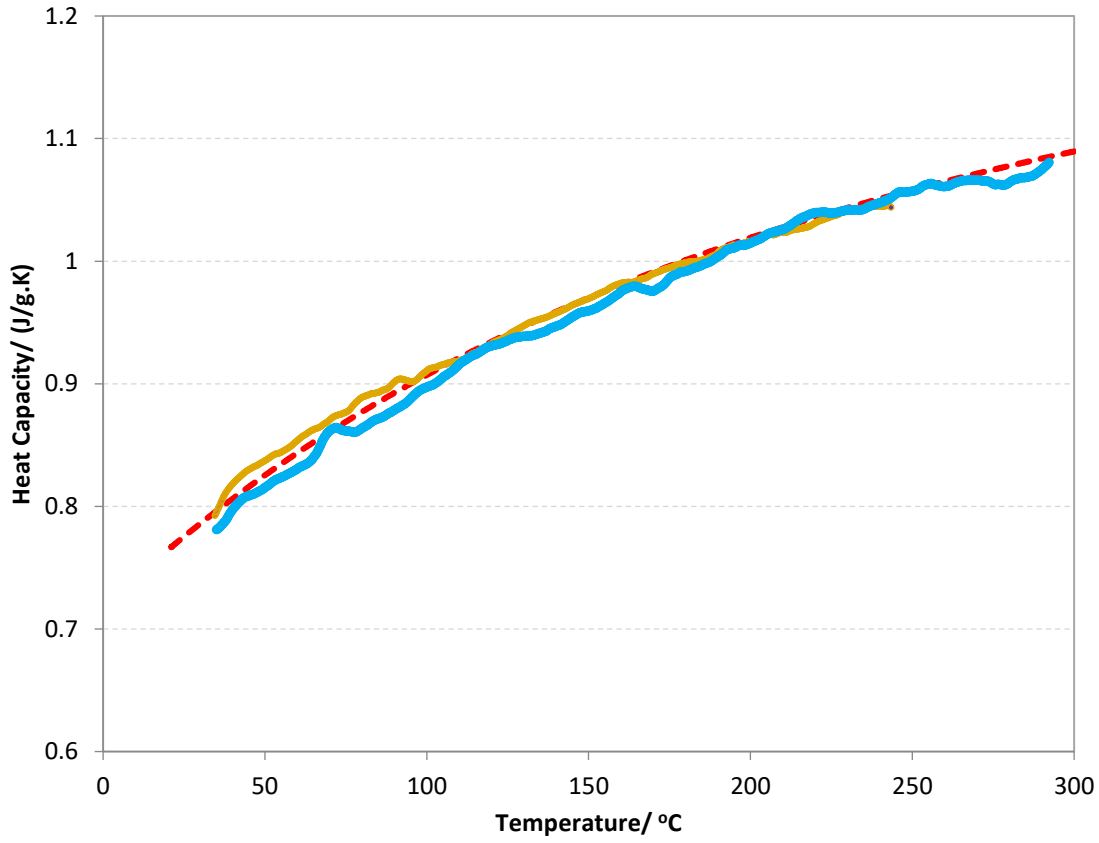


Figure 4. 3:Sapphire heat capacity measured using DSC for the Maltose experiment ---- (blue line) and for the Trehalose experiment --- (orange line), compared to caluclated heat capacity values for sapphire using Archer's equation - - - (Dashed line)

4.2.1.3 Sample Preparation

Glucose, Maltose, Galactose, Trehalose, Saccharine, Aspartame, and Sodium Cyclamate were procured from Sigma-Aldrich. The oxygen mass fraction in these compounds is: 0.53, 0.53, 0.40, 0.53, 0.26, 0.27, and 0.24 respectively. A SARTORIUS CP225D balance, with

an accuracy of 0.01 mg, was used to prepare the samples gravimetrically. Samples weighted 20 -50 mg

4.2.2 Experimental Results

It was difficult to reproduce melting points reported in the literature for sugars. For example, the measured melting temperature for galactose was 451.15 K, determined as shown in Figure 4.4 with its apparent heat capacity shown in Figure 4.5. However, the melting point reported in literature is about 10 degrees lower 437.15 K – 441.15 K[59]. We should note that the tail end of the measured heat capacity profile gives us more insight into the melting temperature of Galactose. In the case of trehalose dihydrate (Figure 4.6) we observed primary melting at around 372 K which is in accordance with literature. As we continued heating the sample, a second melting point was observed at 500K, as opposed to the literature reported number of 478K. Other challenges faced included leaking in the crucibles and caramelization of the sugar outside of the cells. This introduced higher experimental uncertainties between reproduced measurements. Moreover, we observed decomposition of in some of the sugars as well as mass loss during melting. All the experimental sugar melting points can be found in Table 4.3 along with reported values. As for heat capacity data, they can be found in Appendix D, and the heat flow curves in Appendix F. It is evident from the work of Bagheri and Shaw[49], that it is possible that pre-melting phenomena or transitions from solid to liquid crystals are misidentified in prior works or that there are differences in purity. Typically, higher melting temperature values

are more reliable unless heating rates are too high and thermal inertia dominates. No attribution for this outcome is provided at this time.

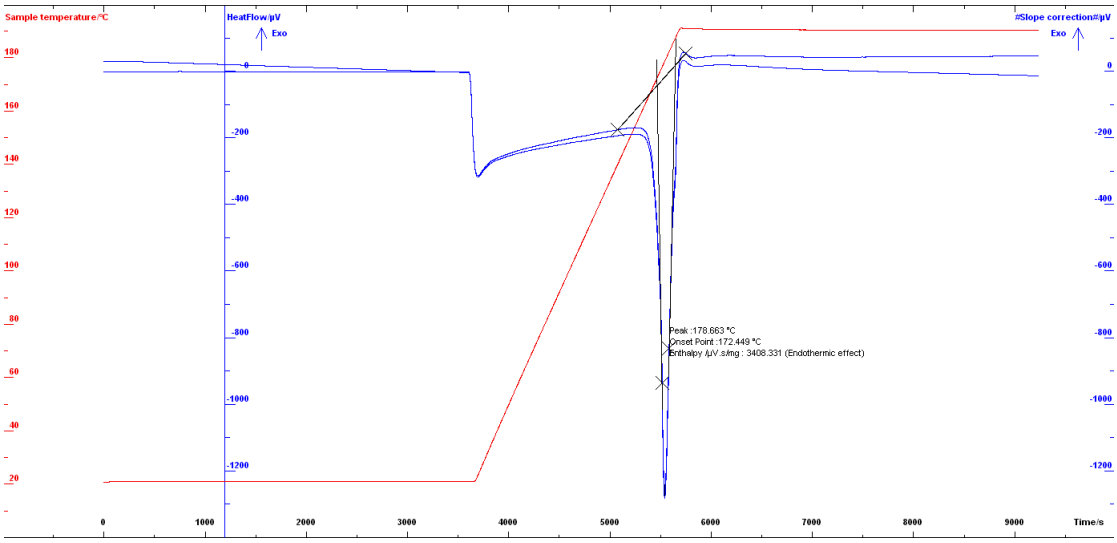


Figure 4. 4:Experimental DSC heat flow curve for Galactose, showing Tm peak at 451.15 K (178 oC)

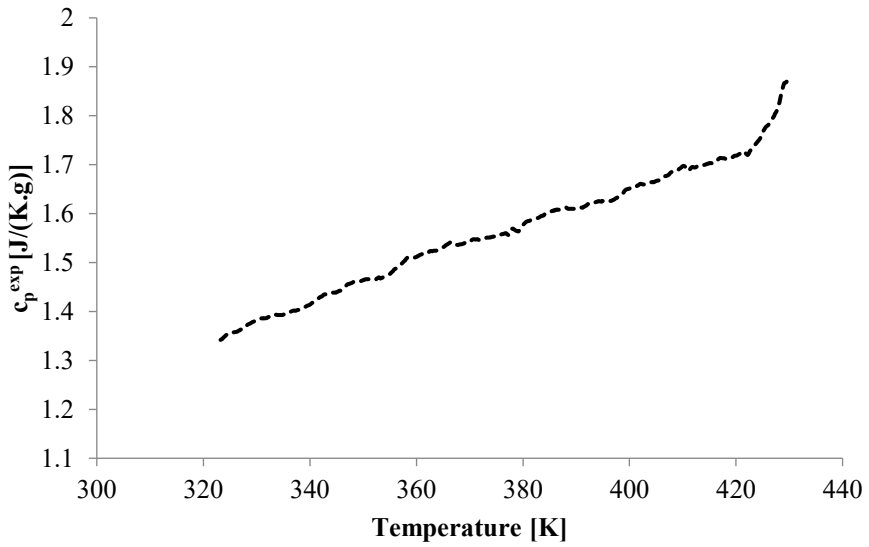


Figure 4. 5:Experimental apparent heat capacity of Galactose

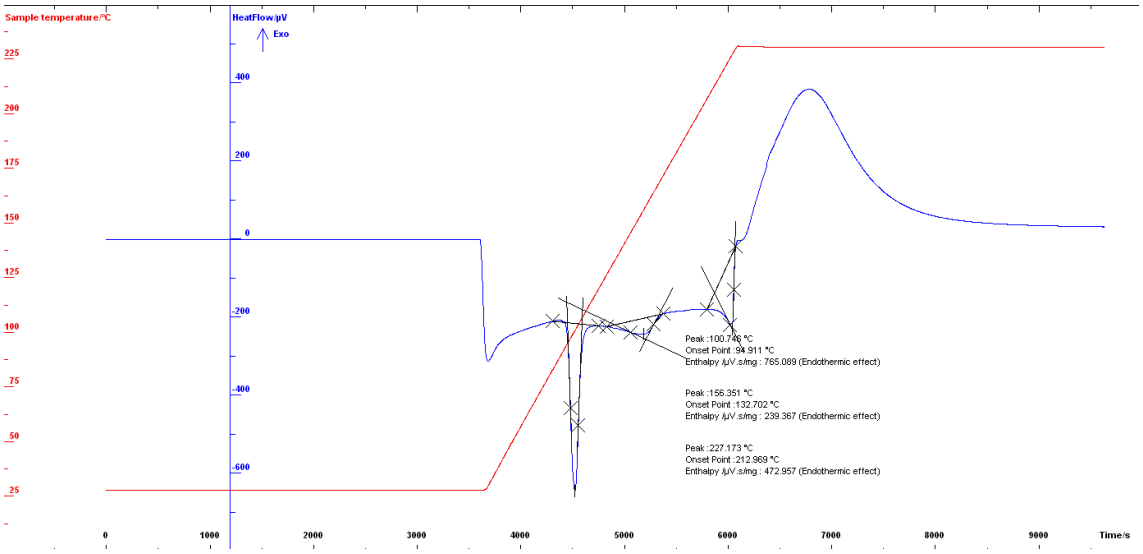


Figure 4. 6:Experimental DSC heat flow curve for Trehalose dihydrate, showing Tm peak at 500 K (227 oC)

Table 4.3: Melting points on the sugar database as measured by the DSC experiments versus the literature reported values

	Purity	**Experimental Melting Point K**	**Reported Melting Point K**
α-D-Glucose , Anhydrous	**>**96%	431	423-425[59]
D-(+)-Maltose monohydrate	>99%	395	375- 376[60]
D-(+)-Trehalose dihydrate	>98.5%	483	476-478[61]
D-(+)-Galactose	>98%	451	437-443[62]
Saccharin	N/A	504	497-503[63]
Sodium Cyclamate	N/A	536	538-573[64]
Aspartame	N/A	493	504-522[65]

4.3 Atom specific adjustment term:

Experimental solid isobaric heat capacities are off-set relative to the correlation (Equation 3-1) and are an increasing function of the heteroatom weight percent (wt.%) as shown in Figures 4.1 and 4.2. For oxygen containing functional groups (Figure 4.1) the nature of the functional group appears immaterial and we can observe a clear positive linear trend between wt.% and increased deviation in c_{pLS} predicted values. For other heteroatoms like Nitrogen (N) and Sulfur (S) they often appeared in the dataset together alongside Oxygen. Due to the small number of data points we could not evaluate the isolated effect of Nitrogen and Sulfur on the deviation. Instead, the weight percent of heteroatom was considered to be a cumulative effect, and it was calculated by including the mass fractions of all three atoms, O, N, and S (Figure 4.2).

A heteroatom specific parameter for solid isobaric heat capacity appears justified, particularly for oxygen. Accordingly, a linear adjustment to the solid correlation was adopted.

$$c_{pALS} = c_{pLS} + aw_{SNO} \tag{4-3}$$

Where,

c_{pALS}*: Adjusted Laštovka -Shaw heat capacity correlation;* $J.K^{-1}.g^{-1}$

c_{pLS}*: Laštovka -Shaw heat capacity correlation;* $J.K^{-1}.g^{-1}$

w_{SNO}*: Mass fraction of heteroatoms, g*

a: regression constant

It should be noted that cyclic carbons where investigated as well but did not yield any positive results.

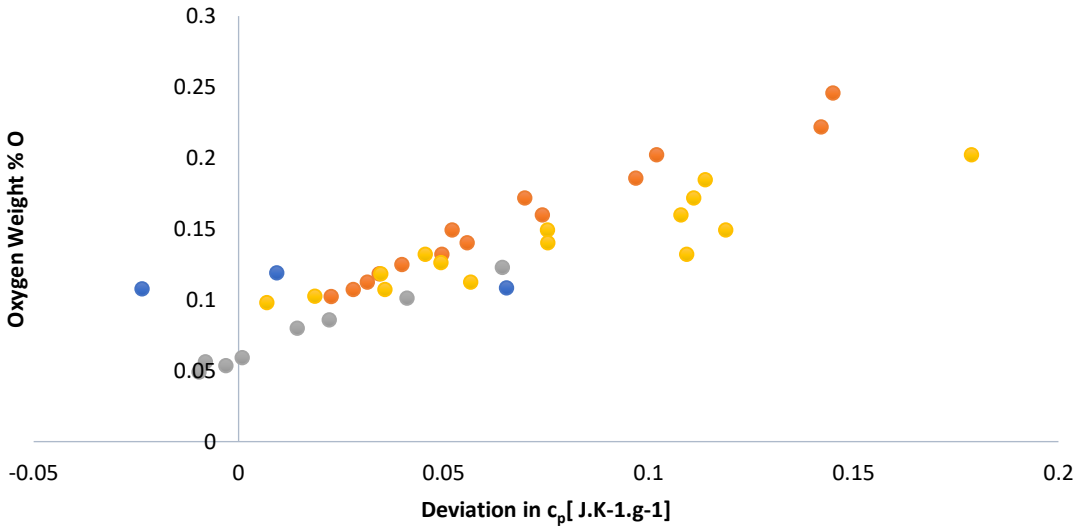


Figure 4. 7:Deviation in predicted values of solid heat capacity from experimental values as a function of weight percent of oxygen for the following chemical families ●Carboxylic Acids ●Triglicerides ● Esters ●Alcohols

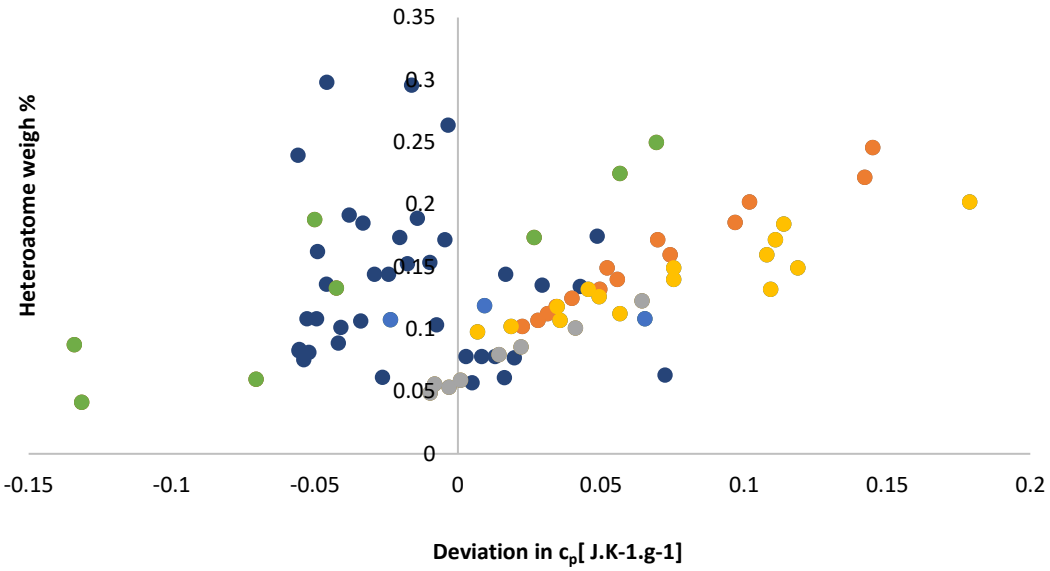


Figure 4. 8:Solid heat capacity differential between experimental and predicted values as a function of weight percent of heteroatoms for the following chemical families ●Carboxylic Acids ●Triglicerides ● Esters ●Alcohols ● Naphthenes ● SNO containing compounds

4.4 Predicting the Heat Capacity of Sugars using the Laštovka -Shaw correlation and the modified Laštovka -Shaw correlation

The Laštovka - Shaw (LS) solid correlation, Equation 3-1, estimates the solid heat capacity of the seven sugars with an absolute relative error of 7.28 % in the test data set. However, with a heteroatom adjusted form (Equation 4-1), trained on heteroatom compounds containing sulfur, oxygen and nitrogen, the absolute relative error drops to 5.43%. Without modification, Equation 3-1, tends to underestimate solid state heat capacities for sugars, seen in Figure 4.9 for Trehalose. The complete list of experimental and calculated sugar isobaric heat capacity data, can be found in Appendix D.

Table 4.4: Absolute error and absolute relative error for the isobaric solid heat capacity correlation, Equation 3-1, and the atom specific adjusted form, Equation 4-1, where a=0.32.

	LS model equation Eq.3-1		Modified LS model equation Eq. 4-1	
Solid	**δ**	**ε**	**δ**	**ε**
Alcohols	0.03	3.02	0.03	3.91
Carboxylic acids	0.06	5.99	0.03	2.99
Esters	0.07	8.13	0.03	3.52
Naphthenes	0.10	11.51	0.10	11.60
SNO	0.04	5.04	0.04	5.66
Triglycerides	0.04	4.64	0.04	5.06
Training Set	**0.06**	**6.68**	**0.05**	**5.46**
Sugars	0.09	7.28	0.09	6.74
Test Set	**0.11**	**7.28**	**0.07**	**5.43**

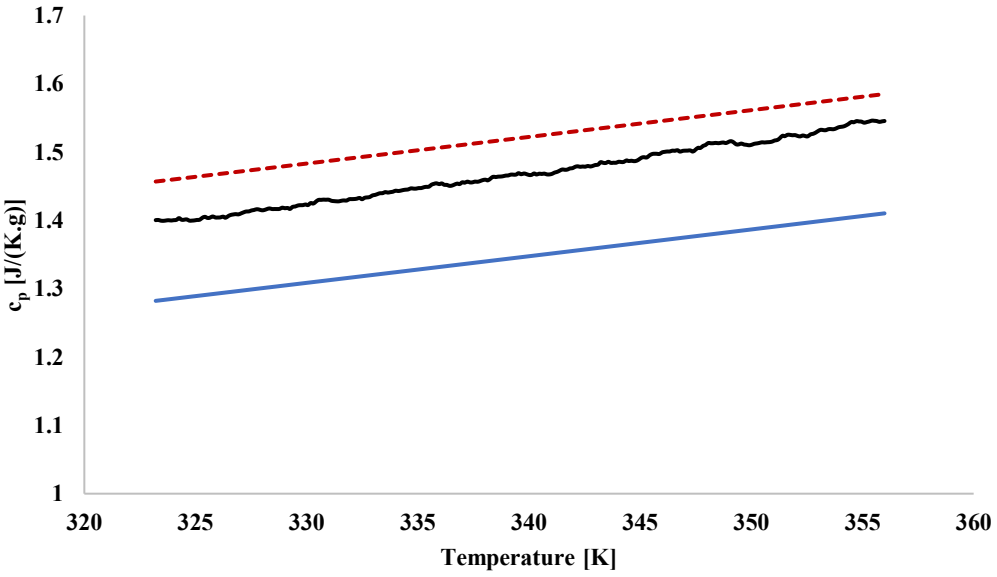


Figure 4. 9:Trehalose solid heat capactity ___cpexp experimental; ___ cpLS (Eq.3-1); _ _ _ cpALS adsjusted LS (Eq.4-1)

Table 4.5: Comparaison of Absolute error and absolute relative error for the isobaric solid heat capacity correlation, Equation 3-1, and the atom specific adjusted form, Equation 4-1, for the sugar database.

	LS model equation Eq.3-1		Modified LS model equation Eq. 4-1	
Sugars	**δ**	**ε.100**	**δ**	**ε.100**
Glucose	0.09	5.83	0.07	4.78
Maltose	0.08	5.17	0.09	6.68

Trehalose	0.12	8.29	0.05	3.61
Galactose	0.08	5.39	0.08	5.36
Saccharine	0.23	16.23	0.04	4.91
Sodium Cyclamate	0.13	8.62	0.05	3.19
Aspartame	0.02	1.48	0.12	9.47

Equation 4-1 yielded better, or similar estimates compared to Equation 3-1, except in the case of Aspartame, where Equation 4-1 overestimated the heat capacity.

4.5 Summary

In this work, we successfully introduced a heteroatom specific modification to the Laštovka - Shaw isobaric heat capacity correlation for organic solids. The added parameter, is only a function of heteroatom weight percent and does not require any further information about compound structure. Isobaric solid heat capacity data of seven sugars, with heteroatom wt% >15, was then measured using a Differential Scanner Calorimeter and served as the test set for correlation validation.

The Laštovka - Shaw correlation (Equation 3-1) and its heteroatom specific modification (Equation 4-1) were successfully extended to estimate the solid isobaric heat capacity of sugars with a heteroatom content up to 53 wt%. Experimental isobaric heat capacity data can vary significantly due to impurities, crystallization and transition phenomena. Both Equations 3-1 and 4-1 provide, easily attainable, c_p estimates for these compounds, at an absolute relative error of less than 8% and 6% respectively.

5 Extending Liquid Isobaric Heat Capacity Correlations to High Hetero Atom Containing Compounds and Mixtures

5.1 Introduction

After extending the solid isobaric heat capacity correlation to better predict compounds with higher heteroatom content like sugars, the same approach was adopted for extending the Dadgostar-Shaw correlation, Equation 3-4, to include high heteroatom containing pure liquids and mixtures such as biodiesels. As with the Laštovka -Shaw correlation for solid isobaric heat capacities, the Dadgostar-Shaw correlation significantly underestimates heat capacity values for compounds and mixtures with high oxygen mass fractions, like biodiesel. An illustrative example is shown in Figures 5.1. Two modifications showed promising results and were explored in detail:

$$c_{pADS} = c_{pDS} + aw_O \tag{5-1}$$

$$c_{pADS} = c_{pDS} + aw_O + bTw_O \tag{5-2}$$

Where,

c_{pADS}*: Adjusted Dadgostar-Shaw heat capacity correlation / J.K*$^{-1}$*.g*$^{-1}$

c_{pDS}*: Dadgostar-Shaw heat capacity correlation / J.K*$^{-1}$*.g*$^{-1}$

w_o*: Mass fraction of oxygen*

a and b: regression constants

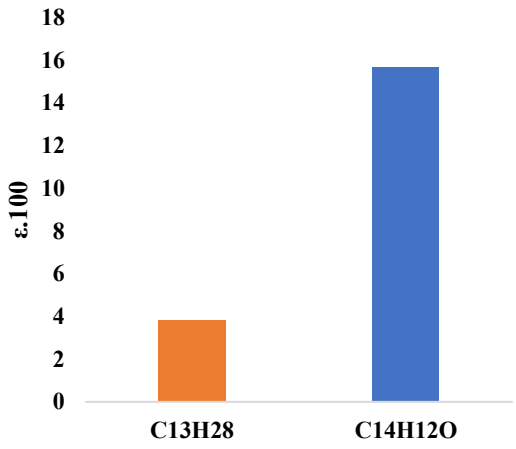


Figure 5. 1:Increase in prediction average absolute deviation for Equation 3-4, for compounds with similar molecular weight, at increased Oxygen wt%

5.2 Characterization Techniques for Biofuels

Biodiesels are complex organic mixtures that can include mono-alkyl esters, glycerol, alcohol, catalyst, free fatty acids, tri-, di- and monoglycerides among their constituents. The most common analytical techniques for characterization are chromatography and spectroscopy[66]. Fatty mono-alkyl ester content, and determination of free and total glycerol are measured industrially as they, along with water content and thermal stability, are indicative of biodiesel quality[67-71]. Biodiesels pyrolyze and care must be taken in interpreting TG, DSC, and DTA curves. They are used to study the stages of thermal decomposition, exothermic transitions, flash points and calorific capacities of biodiesels[70]. For example, Dantas et al.[72] used TG to study the influence of heating rates on the thermogravimetric profile of methyl and ethyl corn biodiesel. Techniques that are currently being used for predicting the liquid heat capacities of biofuels are summarized in Table 5.1. These techniques perform well for mono, di, and tri glycerides and have an average relative error below 3%. However, increased error is observed when estimating values for feed oils.

Zong et al.'s[73] fragment based approach (Equation 5-3) is based on expressing the fragments of triglycerides as a temperature-dependent linear correlation (Equation 5-4). Where N is the number of fragments and $C_{p,A}^{l}$ is the heat capacity contribution of fragment A in (J/Kmol.K). A_1 and A_2 are the parameters of the temperature, T (K), dependent correlation for heat capacity.

$$C_p^l = \sum_A N_{frag,A}\, C_{p,A}^l(T) \tag{5-3}$$

$$C_{p,A}^l = A_{1,A} + A_{2,A}\,(T) \tag{5-4}$$

Ceriani et al,[74] based their approach on a group contribution method. The heat capacity equation (Equation 5-5) was extended from their work on vapour pressure of organic liquids by the addition of a group contribution function in the form of a linear relationship.

$$C_{p_i}^l = \sum_k N_k\,(A_k + B_k.T) \tag{5-5}$$

N_k is the number different groups in a molecule, A_k and B_k are the regression parameters for different groups ie. (CH_3 vs. OH).

As for Morad et al,[75] they developed a two-step method for predicting liquid heat capacity. First, the Rowlinson-Bondi equation (Equation 5-6) is applied to estimate the heat capacity of pure fatty acids. Second a triglyceride-form specific correction factor (Equation 5-12) is applied based on the work done by Halvorsen et al.[76].

$$(C^{l}_{p,FA} - C^{o}_{p,FA})/\,R = 1.45 + 0.45\,(1 - T_r)^{-1} + 0.25\omega\,[17.11 + 25.2(1 - T_r)^{1/3}T_r^{-1} + 1.742(1 - T_r)^{-1}] \quad (5\text{-}6)$$

Cp^l represents specific liquid heat capacity and Cp^o represents ideal gas specific heat capacity.

When dealing with mixtures:

1- Individual fatty acid ideal gas heat capacity is calculated according to the method of Rihani and Doraiswamy[77]:

$$C^{o}_{p_i} = \sum a + \sum bT + \sum cT^2 + \sum dT^3 \quad (5\text{-}7)$$

$$C^{o}_{p,FA} = \sum w_i\, C^{o}_{p_i} \quad (5\text{-}8)$$

2- Reduced temperature is calculated using the specific critical temperature of each fatty acid:

$$T_{c,mix} = \sum w_i\, T_{ci} \quad (5\text{-}9)$$

$$T_r = T/T_{c,mix} \quad (5\text{-}10)$$

3- The acentric factor is also summed based on the fatty acid specific acentric factors:

$$\omega_{mix} = \sum w_i\, \omega_i \quad (5\text{-}11)$$

4- Depending on the molecular weight of the oil, the correction factor is then determined and added to the value calculated from Equation 5-6

$$\mathrm{C}_{p,est} = \mathrm{C}_{p,FA} + \mathrm{F}_c \quad (5\text{-}12)$$

Table 5.1: Existing estimation techniques of isobaric liquid heat capacities of biofuels

Estimation Method	Data Required	Method	Compound Range	Temperature Range (°C)
Zong et al.[73]	Triglyceride of Fatty Acid composition	Fragment-Based Approach	Mono, di, tri - glycerides, DG, MG, feed oil	20 to 180
Ceriani et al.[74]	Fatty Acid composition	Group Contribution	Mono, di, tri - glycerides, DG, MG, feed oil	20 to 250
Morad et al.[75]	Composition, Tci, Fc, Tr, ωi	Rowlinson-Bondi Equation, Group	Triglycerides, feed oil	Tm (melting point) to 250

Experimental feed oil liquid heat capacity data was culled from literature[78]. Predictive methods presented above along with the Dadgostar-Shaw correlation (Equation 3-4) were then used to calculate the isobaric liquid heat capacity and then compared[79]. The results presented in table 5.2, show that that the Dadgostar-Shaw correlation presents a robust, easy to use, and competitive technique for the prediction of isobaric heat capacities of feed oils were simple mixing rules apply. Moreover, it serves as a strong baseline for extension into high heteroatom compound use.

Table 5.2: Absolute relative error for estimated liquid isobaric heat capacities of feed oils[79], using four different techniques.

	%Absolute relative deviation (ε.100)					
	Zong et al.	**Ceriani et al.**		**Morad et al**		**Dadgostar-Shaw (Eq.3-4)**
	Simple TG Approach	**Simple TG Approach**	**Pseudo TG Approach**	**Simple TG Approach**	**Pseudo TG Approach**	
Feed Oils						
Rapeseed	12.14	14.52	14.52	7.3	7.53	11.67
Soybean	12.89	15.42	14.95	6.57	6.88	12.31
Sunflower	9.50	12.41	11.63	2.87	3.07	9.03
Corn	8.01	10.84	10.15	1.81	1.94	5.19
Lard	15.55	17.25	18.66	12.83	13.85	14.41

5.3 Methodology and Biofuel Database

Liquid-state isobaric heat capacities were collected from the work done by Orlando Diaz at the University of Calgary, who collected data using a Differential Scanning Calorimeter (DSC)[80]. The database consisted of seven biofuels: Canola CB-01, Canola I25, Soy MG-B100, Soy SB-100, Rapeseed, Palm oil, and coconut oil. Experimental isobaric heat capacity values were compared to calculated values using the Dadgostar-Shaw predictive correlation for liquids (Equation 4-1) and to its oxygen content corrected forms (Equation 5-1; Equation 5-2).

The liquid isobaric hear capacity's original database (Appendix B) served as the training set and the biofuel database (Appendix E) served as the test set. The coefficients were calculated and tested using multivariate regression tools in MATLAB.

5.4 Results

Equation 3-4 provided a great baseline to fit the data further with a relative absolute error of 8.74 in the tested set. Improved absolute and relative errors where observed when using the two newly proposed forms that include the oxygen mass fraction (Equation 5-1 and 5-2). A slightly better absolute relative error performance of 5.88 was observed when the temperature variable was added in. A general trend of under estimation was observed for all the biofuels. That was mitigated using the adjusted correlation forms as seen in figure 5.2 for Soy S-100.

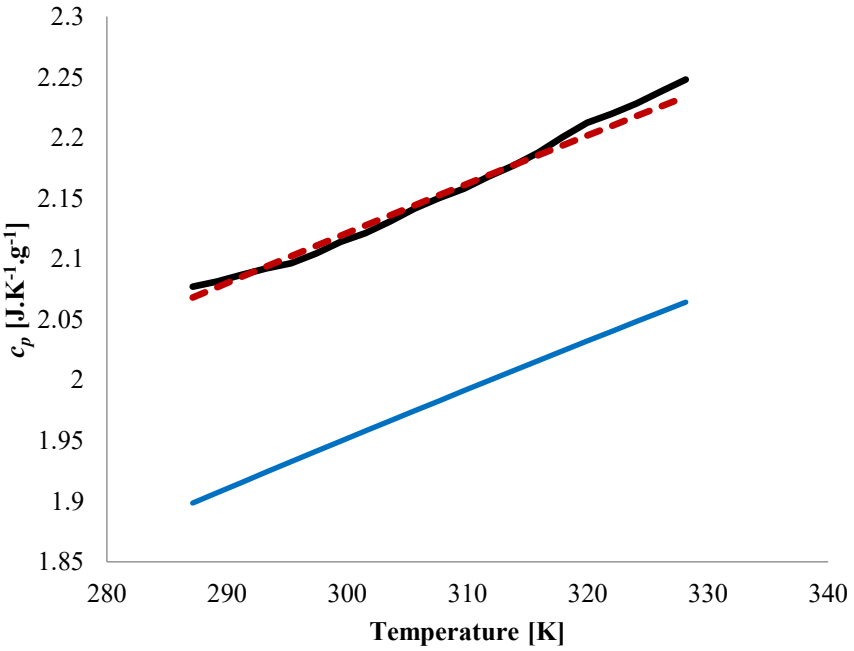


Figure 5. 2:Soy S-100 liquid heat capacity; ___ cpexp experimental [79]; ___ cpDS (Equation 3-4); _ _ _ cpADS adjusted DS(Equation 5-2)

Table 5.3: Absolute and relative error for the isobaric solid heat capacity correlation versus it atom specific adjusted form, where a1=0.45; a2=0.36; b2=0.0004 (Equations 5-1 & 5-2)

	DS model equation Eq.3-4		Modified DS model equation Eq. 5-1		Modified DS model equation Eq. 5-2	
	δ	**ε.100**	**δ**	**ε.100**	**δ**	**ε.100**
Liquids						
SNO	0.11	5.87	0.09	5.04	0.09	4.99
Aromatic	0.10	5.45	N/A	N/A	N/A	N/A
Naphthenes	0.09	4.57	N/A	N/A	N/A	N/A
Maltenes	0.05	2.01	0.07	2.87	0.08	3.31
Training Set	**0.09**	**4.47**	**0.08**	**3.96**	**0.09**	**4.15**
Biofuels	0.19	8.74	0.14	6.24	0.13	5.88
Test Set	**0.19**	**8.74**	**0.14**	**6.24**	**0.13**	**5.88**

5.5 Summary

In this section, we successfully introduced an oxygen specific modification to the Dadgostar-Shaw isobaric heat capacity correlation for organic liquids. The added parameter, is only a function of the oxygen weight percent and/or temperature, and easily calculated from elemental analysis data. Moreover, the Dadgostar-Shaw correlation performance in predicting heat capacities for feed oils was compared to existing predictive techniques for these fluids, and was found to be a competitive and robust option.

The Dadgostar- Shaw correlation (Equation 3-4) and its two modified forms (Equation 5-1 and 5-2) were successfully extended to estimate the liquid isobaric heat capacity of seven biofuels with a heteroatom content around 15 wt.%. All three equations provided c_p estimates for biofuels at an absolute relative error of less than 9% and 7% and 6%, respectively.

6 Conclusions and Recommendations

In the experimental and theoretical work presented in this work, it was demonstrated that the Laštovka -Shaw correlation for solids and the Dadgostar-Shaw correlation for liquids presented a great baseline for the development of high accuracy, family specific heat capacity correlations through numerical modelling (Section 3). For the solid isobaric heat capacity correlation, it's recommended to use the family specific universal coefficients for alkanes, alkenes, alcohols, esters, carboxylic acids and aromatic compounds generated in table 3.3. As for the Liquid isobaric heat capacity correlation it's recommended to use the family specific universal coefficients for alkanes, naphthenes, aromatics and unsaturated cyclics generated in table 3.5.

Numerical manipulation, however, was not the optimal way to tackle compounds with heteroatom content. In developing high precision correlations, the need to accommodate atom type secondary effects became necessary. This prompted the introduction of an enhancement factor that takes into account heteroatom mass fractions (sections 4 and 5). Accordingly, it is recommended to use Equations 4-1 and 5-2 for families containing, sulfur, nitrogen and oxygen.

Moreover, the two correlations were successfully extended to include compounds with high heteroatom content. The solid isobaric heat capacity correlation was extended for sugars (Section 4), and the liquid isobaric heat capacity correlation was extended for biofuels (Section 5). Sugars and Biofuels have >15%wt. of heteroatoms and fall outside of the

recommended range for the use of the similarity variable. However, both original correlations Laštovka -Shaw and Dadgostar-Shaw, performed very well in the prediction of heat capacity of sugars and biofuels, with average relative errors of 8.8 and 7.3 % respectively. These results were comparable to existing techniques, which require a lot more data, making the similarity variable based correlations a successful predictive model even outside of the range it was derived. With this work we were also able to ameliorate these results even further, with the introduction of the enhancement parameter. That lead to a reduction in average relative error to 4.4% for the solid sugar database and to 5.8% for the liquid biofuel database.

Sugars and biofuels, present industrially relevant fluids where thermal stability and thermal properties are integral for process design and optimization. The correlations explored in this work, present an easy, accurate, fast and robust option to determine the heat capacity of these fluids. Unlike existing techniques being used, where calculations can prove laborious and time consuming, and even inaccurate in the case of ill-defined compounds. Thus, it is recommended to extend the use of the similarity variable based correlations to include families of sugars and biofuels. Future work could focus on the extension of this work to other ill -defined industrial fluids that are of interest to the energy and chemical synthesis sectors.

Bibliography

1. Bessières, D., Saint-Guirons, H., and Daridon, J.-L., Measurement and calculation of heat capacity of heavy distillation cuts under pressure up to 40 MPa. Journal of Thermal Analysis and Calorimetry, 1999. 58(1): p. 39-49.

2. Zábranský, M., Růžička, V., and Domalski, E. S., Heat capacity of liquids: Critical review and recommended values. Supplement 1. Journal of Physical and Chemical Reference Data, 2001. 30(5): p. 1199-1689.

3. Smith, J. M., Van Ness, H. C., and Abbott, M. M., Introduction to chemical engineering thermodynamics. 6th ed. McGraw-Hill chemical engineering series. 2001, Boston: McGraw-Hill. xviii, 789 p.

4. Laštovka, V., Prediction of heat capacity of ideal gases and of crystalline phases. Ph.D. Dissertation. 2012, Institute of Chemical Technology (ICT) Prague: Czech Republic.

5. Masliyah, J. H., Xu, Z., Czarnecki, J. A., and Dabros, M., Handbook on theory and practice of bitumen recovery from Athabasca Oil Sands. 2011, Cochrane, Alta.: Kingsley Knowledge Pub.

6. Červinka, C., Fulem, M., Růžička, K., Evaluation of Accuracy of Ideal-Gas Heat Capacity and Entropy Calculations by Density Functional Theory (DFT) for Rigid Molecules. Journal of Chemical & Engineering Data 2012, 57, (1): p. 227-232.

7. Sinha, P., Boesch, S. E., Gu, C. M., Wheeler, R. A., and Wilson, A. K., Harmonic vibrational frequencies: Scaling factors for HF, B3LYP, and MP2 methods in combination with correlation consistent basis sets. Journal of Physical Chemistry A, 2004. 108(42): p. 9213-9217.

8. Laštovka, V. and Shaw, J. M., Predictive correlation for Cp of organic solids based on elemental composition. Journal of Chemical and Engineering Data, 2007. 52(4): p. 1160-1164.

9. Dadgostar, N. and Shaw, J. M., Predictive correlations for liquid heat capacity - including the critical region. Fluid Phase Equilibria, 2013. 344: p. 139-151.

10. Laštovka, V. and Shaw, J. M., Predictive correlations for ideal gas heat capacities of pure hydrocarbons and petroleum fractions. Fluid Phase Equilibria, 2013. 356: p. 338-370.

11. Laštovka, V., Sallamie, N., and Shaw, J. M., A similarity variable for estimating the heat capacity of solid organic compounds - Part I. Fundamentals. Fluid Phase Equilibria, 2008. 268(1-2): p. 51-60.

12. Lappas, A.A., Bezergianni, I.A., and Vasalos, I.A., Production of biofuels via co-processing in conventional refining processes. Catalysis Today, 2009. 2145(1-2): p. 55-62.

13. Goodman, B. T.; Wilding, W. V.; Oscarson, J. L.; Rowley, R. L., Use of the DIPPR Database for Development of Quantitative Structure-Property Relationship Correlations: Heat Capacity of Solid Organic Compounds. Journal of Chemical and Engineering Data 2004, 49, (1): p. 24-31.

14. Chickos, J. S., Hesse, D. G., and Liebman, J. F., A group additivity approach for the estimation of heat capacities of organic liquids and solids at 298 K. Structural Chemistry, 1993. 4(4): p. 261-269.

15. Domalski, E. S. and Hearing, E. D., Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K. Journal of Physical and Chemical Reference Data, 1988. 17(4): p. 1637-1678.

16. Domalski, E. S. and Hearing, E. D., Estimation of the Thermodynamic Properties of C-H-N-O-S-Halogen Compounds at 298.15 K. Journal of Physical and Chemical Reference Data, 1993. 22(4): p. 805-1159.

17. Helgeson, H. C., Owensa, C. E., Knox, A. M., and Richard, L., Calculation of the standard molal thermodynamic properties of crystalline, liquid, and gas organic molecules at high temperatures and pressures. Geochimica Et Cosmochimica Acta, 1998. 62(6): p. 985-1081.

18. Richard, L. and Helgeson, H. C., Calculation of the thermodynamic properties at elevated temperatures and pressures of saturated and aromatic high molecular weight solid and liquid hydrocarbons in kerogen, bitumen, petroleum, and other organic matter of biogeochemical interest. Geochimica Et Cosmochimica Acta, 1998. 62(23-24): p. 3591-3636.

19. Hurst Jr., J. E. and Harrison, B. K., Estimation of liquid and solid heat capacities using a modified Kopp's rule. Chemical Engineering Communications, 1992. 112(1): p. 21-30.

20. Kabo, G. J., Kozyro, A. A., and Diky, V. V., Additivity of Thermodynamic Properties of Organic-Compounds in the Crystalline State .1. Additive Calculations for Thermodynamic Properties of Alkanes, Alkenes, Alkanols, and Alkanones. Journal of Chemical and Engineering Data, 1995. 40(1): p. 160-166.

21. Diky, V. V., Kozyro, A. A., and Kabo, G. J., Additivity of thermodynamic properties of organic compounds in the crystalline state. 3. Heat capacities and related properties of urea phenyl derivatives. Journal of Chemical and Engineering Data, 2002. 47(2): p. 239-244.

22. Briard, A. J., Bouroukba, M.; Petitjean, D., Dirand, M., Models for Estimation of Pure n-Alkanes' Thermodynamic Properties as a Function of Carbon Chain Length. Journal of Chemical and Engineering Data 2003, 48, (6): p. 1508-1516.

23. Reid, R. C. and Sobel, J. E., Estimation of Saturated Liquid Heat Capacities Above Boiling Point. Industrial & Engineering Chemistry Fundamentals, 1965. 4(3): p. 328-331.

24. Poling, B., E., Prausnitz, J., M., and O'Connell, J., P., Thermodynamic Properties of Pure Components and Mixtures, in Properties of Gases and Liquids, Fifth Edition. 2001, McGraw Hill Professional, Access Engineering.

25. Watson, K. M., Thermodynamics of the Liquid State. Industrial & Engineering Chemistry, 1943. 35(4): p. 398-406.

26. Chueh, C. F. and Swanson, A. C., Estimation of Liquid Heat Capacity. Canadian Journal of Chemical Engineering, 1973. 51(5): p. 596-600.

27. Penski, E. C., Chemical Research, D., and Engineering Center Aberdeen Proving Ground, M. D., Estimation of Liquid Heat Capacities. 1. Review and Evaluation of Missenard Method. 1990, Ft. Belvoir: Defense Technical Information Center.

28. Missenard, A., Conductivité thermique des solides, liquides, gaz et de leurs mélanges. 1965, Paris: Eyrolles.

29. Růžička Jr., V. and Domalski, E. S., Estimation of the Heat Capacities of Organic Liquids as a Function of Temperature using Group Additivity. I. Hydrocarbon Compounds. Journal of Physical and Chemical Reference Data, 1993. 22(I3): p. 597-618.

30. Lee, B. I. and Kesler, M. G., Generalized Thermodynamic Correlation Based on 3-Parameter Corresponding States. Aiche Journal, 1975. 21(3): p. 510-527.

31. Rowlinson, J. S. and Watson, I. D., Prediction of thermodynamic properties of fluids and fluid mixtures-I. The principle of corresponding states and its extensions. Chemical Engineering Science, 1969. 24(10): p. 1565-1574.

32. Bondi, A., Estimation of Heat Capacity of Liquids. Industrial & Engineering Chemistry Fundamentals, 1966. 5(4): p. 442-449.

33. Tyagi, K. P., Estimation of saturated liquid heat capacities. Industrial & Engineering Chemistry Process Design and Development, 1975. 14(4): p. 484-488.

34. Stamataki, S. and Tassios, D., Performance of cubic EoS at high pressures. Revue De L Institut Francais Du Petrole, 1998. 53(3): p. 367-377.

35. D. Bessières, H. Saint-Guirons, J.-L. Daridon, J. Thermal Analytical Calorimetry, 1999. 58: p. 39-49

36. Peng, D.-Y. and Robinson, D. B., A New Two-Constant Equation of State. Industrial & Engineering Chemistry Fundamentals, 1976. 15(1): p. 59-64.

37. Robinson, D. B., Peng, D.-Y., and Chung, S. Y.-K., The development of the Peng - Robinson equation and its application to phase-equilibrium in a system containing methanol. Fluid Phase Equilibria, 1985. 24(1-2): p. 25-41.

38. Soave, G., Equilibrium constants from a modified Redlich-Kwong equation of state. Chemical Engineering Science, 1972. 27(6): p. 1197-1203.

39. Péneloux, A., Rauzy, E., and Fréze, R., A consistent correction for Redlich-Kwong-Soave volumes. Fluid Phase Equilibria, 1982. 8(1): p. 7-23.

40. Benedict, M., Webb, G. B., and Rubin, L. C., An Empirical Equation for Thermodynamic Properties of Light Hydrocarbons and Their Mixtures I. Methane, Ethane, Propane and n-Butane. The Journal of Chemical Physics, 1940. 8(4): p. 334-345.

41. Dadgostar, N., Predicting Liquid Phase Heat Capacity of Ill-defined Hydrocarbons. Ph.D Dissertation, in Chemical and Materials Engineering. 2013, University of Alberta: Edmonton, Alberta, Canada.

42. Frenkel, M.; Kabo, G. J.; Marsh, K. N.; Roganov, G. N.; Wilhoit, R. C., Thermodynamics of Organic Compounds in the Gas State, Thermodynamics Research Center: College Station, Texas: 1994; Vol. 1 and 2.

43. Laštovka, V., Fulem, M., Becerra, M., and Shaw, J. M., A similarity variable for estimating the heat capacity of solid organic compounds - Part II. Application: Heat capacity calculation for ill-defined organic solids. Fluid Phase Equilibria, 2008. 268(1-2): p. 134-141.

44. Fulem, M., Laštovka, V., Straka, M., Růžička, K., and Shaw, J. M., Heat capacities of tetracene and pentacene. Journal of Chemical and Engineering Data, 2008. 53(9): p. 2175-2181.

45. Sallamie, N. and Shaw, J. M., Heat capacity prediction for polynuclear aromatic solids using vibration spectra. Fluid Phase Equilibria, 2005. 237(1-2): p. 100-110.

46. Craig, D. Q. M., Pharmaceutical Applications of DSC, in Thermal Analysis of Pharmaceuticals. 2006, CRC Press. p. 53-99.

47. Craig, D. Q. M. and Galwey, A. K., Thermogravimetric Analysis: Pharmaceutical Applications, in Thermal Analysis of Pharmaceuticals. 2006, CRC Press. p. 193-219.

48. Lee, J. W., Investigation of thermal decomposition as the cause of the loss of crystalline structure in sucrose, glucose, and fructose. Ph.D. Dissertation. 2010, University of Illinois at Urbana-Champaign: Illinois, US.

49. Bagheri, S. R. and Shaw, J. M., Observation of Liquid-Crystal Formation during Melting of D-(+)-Glucose. Journal of Agricultural and Food Chemistry, 2011. 59(23): p. 12605-12609.

50. Höhne, G., Hemminger, W., and Flammersheim, H. J., Differential scanning calorimetry. 2003, Springer: Berlin, Germany

51. Kett, V. L., Murphy, J. R., Craig, D. Q. M., and Reading, M., Modulated Temperature Differential Scanning Calorimetry, in Thermal Analysis of Pharmaceuticals. 2006, CRC Press. p. 101-138.

52. Marini, A., Berbenni, V., Flor, G., Massarotti, V., and Riccardi, R., An analysis of the factors affecting the peak shape and the quantitative reliability of a heat flux DSC cell. Thermochimica Acta, 1985. 95(2): p. 419-424.

53. Diedrichs, A. and Gmehling, J., Measurement of heat capacities of ionic liquids by differential scanning calorimetry. Fluid Phase Equilibria, 2006. 244(1): p. 68-77.

54. Gmelin, E. and Sarge, S. M., Temperature, heat and heat flow rate calibration of differential scanning calorimeters. Thermochimica Acta, 2000. 347(1): p. 9-13.

55. Sabbah, R., Xu-wu, A., Chickos, J. S., Leitão, M. L. P., Roux, M. V., and Torres, L. A., Reference materials for calorimetry and differential thermal analysis. Thermochimica Acta, 1999. 331(2): p. 93-204.

56. Chirico, R. D., Knipmeyer, S. E., Nguyen, A., and Steele, W. V., The thermodynamic properties of biphenyl. The Journal of Chemical Thermodynamics, 1989. 21(12): p. 1307-1331.

57. Finke, H. L., Messerly, J. F., Lee, S. H., Osborn, A. G., and Douslin, D. R., Comprehensive thermodynamic studies of seven aromatic hydrocarbons. The Journal of Chemical Thermodynamics, 1977. 9(10): p. 937-956.

58. Knothe, G., Analytical methods used in the production and fuel quality assessment of biodiesel. Transactions of the Asae, 2001. 44(2): p. 193-200.

59. Jónsdóttir, Svava Ósk; Cooke, Stephen A.; Macedo, Eugénia A., Modeling and measurements of solid--liquid and vapor--liquid equilibria of polyols and carbohydrates in aqueous solution, Carbohydrate Research, 2002. 337(17): p. 1563-1571.

60. Parks, G.S., Thomas, S.B., The heat capacities of crystalline, glassy and undercooled liquid glucose, J. Am. Chem. Soc., 1934. 52: p. 1423

61. NIST Standard Reference Database 203 Web Thermo Tables, 2017 [Online]. Available: http://wtt-pro.nist.gov/wtt-pro/index.html?cmp=alpha.alpha-trehalose

62. Taylor, L.S., York P., Charaterization of the phase transitions of trehalose dihydrate on heating and subsequent dehydration, J. Pharm. Sci., 1998. 87(3): p.347-355

63. Good, David J.; Rodriguez-Hornedo, Nair, Solubility Advantage of Pharmaceutical Cocrystals, Crystal Growth & Design, 2009. 9(5): p: 2252-2264.

64. U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID6020355 (accessed November 15, 2017), Sodium cyclamate

65. Schlatter, J.M.; US.Patent 3,492,131; January 27, 1970; assigned to G.D. Searle & Co.

66. Conceição, M. M., Candeia, R. A., Silva, F. C., Bezerra, A. F., Fernandes, V. J., and Souza, A. G., Thermoanalytical characterization of castor oil biodiesel. Renewable and Sustainable Energy Reviews, 2007. 11(5): p. 964-975

67. Plank, C. and Lorbeer, E., Simultaneous determination of glycerol, and mono-, di- and triglycerides in vegetable oil methyl esters by capillary gas chromatography. Journal of Chromatography A, 1995. 697(1): p. 461-468.

68. Wawrzyniak, R. and Wasiak, W., Determination of acylglycerols in diesel oils by GC. Toxicology Mechanisms and Methods, 2008. 18(6): p. 531-536.

69. Wawrzyniak, R., Wasiak, W., and Frackowiak, M., Determination of methyl esters in diesel oils by gas chromatography - Validation of the method. Chemical Papers, 2005. 59(6B): p. 449-452.

70. Monteiro, M. R., Ambrozin, A. R. P., Liao, L. M., and Ferreira, A. G., Critical review on analytical methods for biodiesel characterization. Talanta, 2008. 77(2): p. 593-605.

71. Santos, N. A., Tavares, M. L. A., Rosenhaim, R., Silva, F. C., Fernandes, V. J., Santos, I. M. G., and Souza, A. G., Thermogravimetric and calorimetric evaluation of babassu

biodiesel obtained by the methanol route. Journal of Thermal Analysis and Calorimetry, 2007. 87(3): p. 649-652.

72. Dantas, M. B., Almeida, A. A. F., Conceicao, M. M., Fernandes, V. J., Santos, I. M. G., Silva, F. C., Soledade, L. E. B., and Souza, A. G., Characterization and kinetic compensation effect of corn biodiesel. Journal of Thermal Analysis and Calorimetry, 2007. 87(3): p. 847-851.

73. Zong, L., Ramanathan, S., and Chen, C. C., Fragment-Based Approach for Estimating Thermophysical Properties of Fats and Vegetable Oils for Modeling Biodiesel Production Processes. Industrial & Engineering Chemistry Research, 2010. 49(2): p. 876-886.

74. Ceriani, R., Gani, R., and Meirelles, A. J. A., Prediction of heat capacities and heats of vaporization of organic liquids by group contribution methods. Fluid Phase Equilibria, 2009. 283(1-2): p. 49-55.

75. Morad, N. A., Kamal, A. A. M., Panau, F., and Yew, T. W., Liquid specific heat capacity estimation for fatty acids, triacylglycerols, and vegetable oils based on their fatty acid composition. Journal of the American Oil Chemists Society, 2000. 77(9): p. 1001-1005.

76. Halvorsen, J. D., Mammel, W. C., and Clements, L. D., Density estimation for fatty acids and vegetable oils based on their fatty acid composition. Journal of the American Oil Chemists Society, 1993. 70(9): p. 875-880.

77. Rihani, D. N. and Doraiswamy, L. K., Estimation of heat capacity of organic compounds from group contributions. Industrial & Engineering Chemistry Fundamentals, 1965. 4(1): p. 17-+.

78. Kowalski, B., Determination of specific heats of some edible oils and fats by differential scanning calorimetry. Journal of Thermal Analysis, 1988. 34(5-6): p. 1321-1326.

79. Su, Y. C., Liu, Y. A., Diaz Tovar, C. A., and Gani, R., Selection of Prediction Methods for Thermophysical Properties for Process Modeling and Product Design of Biodiesel Manufacturing. Industrial & Engineering Chemistry Research, 2011. 50(11): p. 6809-6836.

80. Castellanos Díaz, O., Measurement And Modelling Methodology For Heavy Oil And Bitumen Vapour Pressure. Ph.D Dissertation. 2012, University of Calgary: Calgary, Alberta, Canada.

Appendix A: Solid Isobaric Heat Capacity Database

Name	Formula	M [g.mol^{-1}]	α [mol.g^{-1}]	Database	T [K]	C_{pLS} [J.K^{-1}.g^{-1}]			
						Experimental	Calculated using Lastovka-Shaw (LS) Equation 3-1	Calculated using the adjusted LS Table 3.3	Calculated using the heteroatom correctedLS Equation 4-1
Alkanes									
Nonane	C9H20	128.26	0.226	Test set 1, Training set 2	50.00	0.456	0.426	0.426	0.426
					60.00	0.559	0.517	0.517	0.517
					70.00	0.648	0.596	0.596	0.596
					80.00	0.730	0.667	0.666	0.667
					90.00	0.805	0.731	0.730	0.731
					100.00	0.869	0.791	0.790	0.791
					110.00	0.929	0.847	0.847	0.847
					120.00	0.986	0.902	0.901	0.902
					130.00	1.040	0.954	0.953	0.954
					140.00	1.092	1.005	1.004	1.005

					150.00	1.142	1.055	1.054	1.055
					160.00	1.193	1.104	1.103	1.104
					170.00	1.246	1.152	1.151	1.152
					180.00	1.303	1.200	1.199	1.200
					190.00	1.367	1.247	1.246	1.247
2-Methylnonane	C10H22	142.28	0.225	Test set 1, Training set 2	80.00	0.735	0.663	0.662	0.663
					90.00	0.799	0.727	0.726	0.727
					100.00	0.863	0.786	0.786	0.786
					110.00	0.925	0.843	0.842	0.843
					120.00	0.983	0.897	0.896	0.897
					130.00	1.036	0.949	0.948	0.949
					140.00	1.088	1.000	0.999	1.000
					150.00	1.140	1.049	1.049	1.049
					160.00	1.192	1.098	1.097	1.098
					170.00	1.264	1.146	1.146	1.146
3-Methylnonane	C10H22	142.28	0.225	Test set 1, Training set 2	80.00	0.708	0.663	0.662	0.663
					90.00	0.773	0.727	0.726	0.727
					100.00	0.837	0.786	0.786	0.786
					110.00	0.898	0.843	0.842	0.843

					120.00	0.956	0.897	0.896	0.897
					130.00	1.015	0.949	0.948	0.949
					140.00	1.072	1.000	0.999	1.000
					150.00	1.125	1.049	1.049	1.049
					160.00	1.173	1.098	1.097	1.098
					170.00	1.246	1.146	1.146	1.146
5-Methylnonane	C10H22	142.28	0.225	Test set 1, Training set 2	80.00	0.731	0.663	0.662	0.663
					90.00	0.799	0.727	0.726	0.727
					100.00	0.861	0.786	0.786	0.786
					110.00	0.921	0.843	0.842	0.843
					120.00	0.979	0.897	0.896	0.897
					130.00	1.037	0.949	0.948	0.949
					140.00	1.090	1.000	0.999	1.000
					150.00	1.142	1.049	1.049	1.049
					160.00	1.197	1.098	1.097	1.098
					170.00	1.287	1.146	1.146	1.146
					50.00	0.440	0.423	0.423	0.423
					60.00	0.540	0.514	0.513	0.514
					70.00	0.629	0.593	0.592	0.593

Decane	C10H22	142.28	0.225	Test set 1, Training set 2	80.00	0.708	0.663	0.662	0.663
					90.00	0.779	0.727	0.726	0.727
					100.00	0.841	0.786	0.786	0.786
					110.00	0.898	0.843	0.842	0.843
					120.00	0.953	0.897	0.896	0.897
					130.00	1.005	0.949	0.948	0.949
					140.00	1.054	1.000	0.999	1.000
					150.00	1.102	1.049	1.049	1.049
					160.00	1.148	1.098	1.097	1.098
					170.00	1.195	1.146	1.146	1.146
					180.00	1.244	1.194	1.193	1.194
					190.00	1.295	1.241	1.240	1.241
					200.00	1.348	1.288	1.287	1.288
					210.00	1.406	1.334	1.333	1.334
Undecane	C11H24	156.31	0.224	Test set 1, Training set 2	50.00	0.428	0.421	0.421	0.421
					60.00	0.528	0.511	0.511	0.511
					70.00	0.618	0.590	0.589	0.590
					80.00	0.698	0.659	0.659	0.659
					90.00	0.771	0.723	0.722	0.723

					100.00	0.834	0.783	0.782	0.783
					110.00	0.892	0.839	0.838	0.839
					120.00	0.946	0.893	0.892	0.893
					130.00	0.998	0.945	0.944	0.945
					140.00	1.047	0.995	0.994	0.995
					150.00	1.095	1.045	1.044	1.045
					160.00	1.142	1.094	1.093	1.094
					170.00	1.192	1.142	1.141	1.142
					180.00	1.243	1.189	1.188	1.189
					190.00	1.297	1.236	1.235	1.236
					200.00	1.356	1.283	1.282	1.283
					210.00	1.421	1.329	1.328	1.329
					220.00	1.494	1.375	1.374	1.375
Dodecane	C12H26	170.33	0.223	Test set 1, Training set 2	50.00	0.418	0.419	0.419	0.419
					60.00	0.518	0.509	0.509	0.509
					70.00	0.605	0.587	0.587	0.587
					80.00	0.684	0.657	0.656	0.657
					90.00	0.755	0.720	0.719	0.720
					100.00	0.815	0.779	0.779	0.779

					110.00	0.871	0.835	0.835	0.835
					120.00	0.924	0.889	0.888	0.889
					130.00	0.974	0.941	0.940	0.941
					140.00	1.022	0.992	0.991	0.992
					150.00	1.067	1.041	1.040	1.041
					160.00	1.112	1.090	1.089	1.090
					170.00	1.157	1.138	1.137	1.138
					180.00	1.205	1.185	1.185	1.185
					190.00	1.252	1.232	1.231	1.232
					200.00	1.302	1.279	1.278	1.279
					210.00	1.355	1.325	1.324	1.325
					220.00	1.411	1.371	1.370	1.371
					230.00	1.474	1.417	1.416	1.417
					50.00	0.410	0.418	0.417	0.418
					60.00	0.510	0.507	0.507	0.507
					70.00	0.599	0.585	0.584	0.585
					80.00	0.679	0.654	0.654	0.654
					90.00	0.750	0.718	0.717	0.718
					100.00	0.812	0.777	0.776	0.777

Tridecane	C13H28	184.36	0.222	Test set 1, Training set 2	110.00	0.869	0.833	0.832	0.833
					120.00	0.923	0.886	0.885	0.886
					130.00	0.974	0.938	0.937	0.938
					140.00	1.022	0.989	0.988	0.989
					150.00	1.069	1.038	1.037	1.038
					160.00	1.115	1.087	1.086	1.087
					170.00	1.160	1.135	1.134	1.135
					180.00	1.208	1.182	1.181	1.182
					190.00	1.258	1.229	1.228	1.229
					200.00	1.311	1.275	1.275	1.275
					210.00	1.369	1.322	1.321	1.322
					220.00	1.434	1.368	1.367	1.368
Tetradecane	C14H30	198.39	0.222	Training set 1, Training set 2	50.00	0.402	0.417	0.416	0.417
					60.00	0.501	0.506	0.505	0.506
					70.00	0.588	0.583	0.582	0.583
					80.00	0.667	0.652	0.652	0.652
					90.00	0.736	0.716	0.715	0.716
					100.00	0.795	0.774	0.773	0.774
					110.00	0.851	0.830	0.829	0.830

					120.00	0.903	0.884	0.883	0.884
					130.00	0.952	0.936	0.935	0.936
					140.00	0.998	0.986	0.985	0.986
					150.00	1.044	1.035	1.034	1.035
					160.00	1.088	1.084	1.083	1.084
					170.00	1.133	1.132	1.131	1.132
					180.00	1.178	1.179	1.178	1.179
					190.00	1.224	1.226	1.225	1.226
					200.00	1.272	1.273	1.272	1.273
					210.00	1.321	1.319	1.318	1.319
					220.00	1.374	1.365	1.363	1.365
Pentadecane	C15H32	212.41	0.221	Training set 1, Training set 2	50.00	0.397	0.415	0.415	0.415
					60.00	0.495	0.504	0.504	0.504
					70.00	0.583	0.582	0.581	0.582
					80.00	0.662	0.651	0.650	0.651
					90.00	0.733	0.714	0.713	0.714
					100.00	0.793	0.772	0.771	0.772
					110.00	0.850	0.828	0.827	0.828
					120.00	0.903	0.882	0.881	0.882

					130.00	0.953	0.933	0.932	0.933
					140.00	1.000	0.984	0.983	0.984
					150.00	1.046	1.033	1.032	1.033
					160.00	1.091	1.082	1.081	1.082
					170.00	1.136	1.129	1.128	1.129
					180.00	1.182	1.177	1.176	1.177
					190.00	1.229	1.224	1.223	1.224
					200.00	1.279	1.270	1.269	1.270
					210.00	1.331	1.316	1.315	1.316
Hexadecane	C16H34	226.44	0.221	Training set 1, Training set 2	50.00	0.390	0.414	0.414	0.414
					60.00	0.489	0.503	0.502	0.503
					70.00	0.574	0.580	0.579	0.580
					80.00	0.652	0.649	0.648	0.649
					90.00	0.722	0.712	0.711	0.712
					100.00	0.781	0.771	0.770	0.771
					110.00	0.836	0.826	0.825	0.826
					120.00	0.887	0.880	0.879	0.880
					130.00	0.935	0.931	0.930	0.931
					180.00	1.157	1.175	1.174	1.175

					190.00	1.203	1.221	1.220	1.221
					200.00	1.250	1.268	1.267	1.268
					210.00	1.299	1.314	1.313	1.314
					220.00	1.351	1.360	1.359	1.360
Heptadecane	C17H36	240.47	0.220	Training set 1, Training set 2	50.00	0.387	0.413	0.413	0.413
					60.00	0.486	0.502	0.501	0.502
					70.00	0.572	0.579	0.578	0.579
					80.00	0.650	0.648	0.647	0.648
					90.00	0.721	0.711	0.710	0.711
					100.00	0.780	0.769	0.768	0.769
					110.00	0.836	0.825	0.824	0.825
					120.00	0.888	0.878	0.877	0.878
					130.00	0.937	0.930	0.929	0.930
					140.00	0.984	0.980	0.979	0.980
					150.00	1.029	1.029	1.028	1.029
					160.00	1.074	1.078	1.077	1.078
					170.00	1.118	1.125	1.124	1.125
					180.00	1.164	1.173	1.172	1.173
					190.00	1.210	1.219	1.218	1.219

					200.00	1.258	1.266	1.265	1.266
					210.00	1.309	1.312	1.311	1.312
					220.00	1.364	1.358	1.357	1.358
Octadecane	C18H38	254.49	0.220	Training set 1, Training set 2	50.00	0.378	0.413	0.412	0.413
					60.00	0.479	0.501	0.500	0.501
					70.00	0.566	0.578	0.577	0.578
					80.00	0.643	0.646	0.646	0.646
					90.00	0.712	0.709	0.708	0.709
					100.00	0.770	0.768	0.767	0.768
					110.00	0.825	0.823	0.822	0.823
					120.00	0.876	0.877	0.876	0.877
					130.00	0.924	0.928	0.927	0.928
					140.00	0.970	0.978	0.977	0.978
					150.00	1.013	1.028	1.026	1.028
					160.00	1.057	1.076	1.075	1.076
					170.00	1.100	1.124	1.123	1.124
					180.00	1.143	1.171	1.170	1.171
					190.00	1.188	1.218	1.217	1.218
					200.00	1.233	1.264	1.263	1.264

					210.00	1.280	1.310	1.309	1.310
					220.00	1.331	1.356	1.355	1.356
Nonadecane	C19H40	268.52	0.220	Training set 1, Training set 2	50.00	0.380	0.412	0.411	0.412
					55.00	0.429	0.458	0.457	0.458
					60.00	0.477	0.500	0.499	0.500
					65.00	0.522	0.540	0.539	0.540
					70.00	0.565	0.577	0.576	0.577
					75.00	0.603	0.612	0.611	0.612
					80.00	0.640	0.645	0.645	0.645
					85.00	0.675	0.677	0.676	0.677
					90.00	0.708	0.708	0.707	0.708
					95.00	0.740	0.738	0.737	0.738
					100.00	0.769	0.767	0.766	0.767
					105.00	0.798	0.795	0.794	0.795
					110.00	0.825	0.822	0.821	0.822
					120.00	0.877	0.875	0.874	0.875
					130.00	0.925	0.927	0.926	0.927
					140.00	0.971	0.977	0.976	0.977
					150.00	1.015	1.026	1.025	1.026

					160.00	1.059	1.074	1.073	1.074
					170.00	1.105	1.122	1.121	1.122
					180.00	1.150	1.169	1.168	1.169
					190.00	1.196	1.216	1.215	1.216
					200.00	1.245	1.263	1.261	1.263
					210.00	1.294	1.309	1.307	1.309
					220.00	1.347	1.354	1.353	1.354
					230.00	1.403	1.400	1.399	1.400
					50.00	0.377	0.411	0.411	0.411
					55.00	0.425	0.457	0.456	0.457
					60.00	0.473	0.499	0.499	0.499
					65.00	0.518	0.539	0.538	0.539
					70.00	0.560	0.576	0.575	0.576
					75.00	0.598	0.611	0.610	0.611
					80.00	0.634	0.644	0.644	0.644
					85.00	0.669	0.676	0.676	0.676
					90.00	0.702	0.707	0.706	0.707
					95.00	0.733	0.737	0.736	0.737
					100.00	0.762	0.765	0.765	0.765

Eicosane	C20H42	282.55	0.219	Test set 1, Training set 2	105.00	0.790	0.793	0.793	0.793
					110.00	0.817	0.821	0.820	0.821
					120.00	0.866	0.874	0.873	0.874
					130.00	0.914	0.925	0.925	0.925
					140.00	0.959	0.976	0.975	0.976
					150.00	1.002	1.025	1.024	1.025
					160.00	1.044	1.073	1.072	1.073
					170.00	1.087	1.121	1.120	1.121
					180.00	1.130	1.168	1.167	1.168
					190.00	1.174	1.215	1.214	1.215
					200.00	1.220	1.261	1.260	1.261
					210.00	1.267	1.307	1.306	1.307
					220.00	1.317	1.353	1.352	1.353
					230.00	1.369	1.398	1.397	1.398
					240.00	1.425	1.444	1.443	1.444
					250.00	1.481	1.489	1.488	1.489
					260.00	1.542	1.533	1.532	1.533
					270.00	1.609	1.578	1.577	1.578
					80.00	0.627	0.641	0.641	0.641

Tetracosane	C24H50	338.659	0.219	Test set 1, Training set 2	90.00	0.692	0.704	0.703	0.704
					100.00	0.753	0.762	0.761	0.762
					110.00	0.810	0.817	0.816	0.817
					120.00	0.861	0.870	0.869	0.870
					130.00	0.906	0.922	0.921	0.922
					140.00	0.946	0.972	0.971	0.972
					150.00	0.987	1.021	1.020	1.021
					160.00	1.031	1.069	1.068	1.069
					170.00	1.080	1.117	1.116	1.117
					180.00	1.132	1.164	1.163	1.164
					190.00	1.182	1.210	1.209	1.210
					200.00	1.233	1.257	1.256	1.257
					210.00	1.286	1.303	1.302	1.303
					220.00	1.351	1.348	1.347	1.348
					230.00	1.421	1.394	1.393	1.394
					240.00	1.498	1.439	1.438	1.439
					250.00	1.598	1.484	1.483	1.484
Pentacosane	C25H52	326.45	0.218	Test set 1, Training set 2	91.30	0.703	0.711	0.710	0.711
					97.80	0.736	0.749	0.748	0.749

					122.70	0.858	0.883	0.883	0.883
					152.00	0.992	1.030	1.029	1.030
					180.30	1.142	1.164	1.163	1.164
					194.50	1.222	1.230	1.229	1.230
					199.90	1.255	1.255	1.254	1.255
					223.50	1.397	1.363	1.362	1.363
					240.70	1.510	1.441	1.440	1.441
					50.00	0.368	0.409	0.408	0.409
					60.00	0.463	0.496	0.495	0.496
					70.00	0.547	0.572	0.571	0.572
					80.00	0.621	0.640	0.639	0.640
					90.00	0.686	0.702	0.702	0.702
					100.00	0.745	0.761	0.760	0.761
					110.00	0.799	0.816	0.815	0.816
					120.00	0.849	0.869	0.868	0.869
					130.00	0.895	0.920	0.919	0.920
					140.00	0.938	0.970	0.969	0.970
					150.00	0.980	1.019	1.018	1.019
					160.00	1.021	1.067	1.066	1.067

Hexacosane	C26H54	366.713	0.218	Test set 1, Training set 2	170.00	1.063	1.115	1.114	1.115
					180.00	1.106	1.162	1.161	1.162
					190.00	1.150	1.209	1.208	1.209
					200.00	1.195	1.255	1.254	1.255
					210.00	1.241	1.301	1.300	1.301
					220.00	1.289	1.347	1.346	1.347
					230.00	1.340	1.392	1.391	1.392
					240.00	1.394	1.437	1.436	1.437
					250.00	1.452	1.482	1.481	1.482
					260.00	1.513	1.527	1.526	1.527
11-Decylheneicosane	C31H64	436.84	0.217		50.00	0.389	0.407	0.407	0.407
					60.00	0.474	0.494	0.493	0.494
					70.00	0.552	0.570	0.569	0.570
					80.00	0.622	0.638	0.637	0.638
					90.00	0.684	0.700	0.699	0.700
					100.00	0.740	0.758	0.757	0.758
					110.00	0.789	0.813	0.812	0.813
					120.00	0.834	0.866	0.865	0.866
					130.00	0.879	0.917	0.916	0.917

				Test set 1, Training set 2	140.00	0.923	0.967	0.966	0.967
					150.00	0.967	1.016	1.015	1.016
					160.00	1.011	1.064	1.063	1.064
					170.00	1.057	1.112	1.111	1.112
					180.00	1.105	1.159	1.158	1.159
					190.00	1.154	1.205	1.204	1.205
					200.00	1.206	1.252	1.251	1.252
					210.00	1.264	1.297	1.296	1.297
					220.00	1.324	1.343	1.342	1.343
					230.00	1.389	1.389	1.388	1.389
					240.00	1.462	1.434	1.433	1.434
					250.00	1.534	1.479	1.478	1.479
					260.00	1.605	1.524	1.522	1.524
					265.00	1.640	1.546	1.545	1.546
Dotriacontane	C32H66	450.873	0.217	Test set 1, Training set 2	80.00	0.618	0.638	0.637	0.638
					90.00	0.675	0.700	0.699	0.700
					100.00	0.730	0.758	0.757	0.758
					110.00	0.785	0.813	0.812	0.813
					120.00	0.838	0.865	0.865	0.865

					130.00	0.890	0.917	0.916	0.917
					140.00	0.932	0.967	0.966	0.967
					150.00	0.971	1.015	1.015	1.015
					160.00	1.011	1.064	1.063	1.064
					170.00	1.056	1.111	1.110	1.111
					180.00	1.104	1.158	1.157	1.158
					190.00	1.154	1.205	1.204	1.205
					200.00	1.207	1.251	1.250	1.251
					210.00	1.268	1.297	1.296	1.297
					220.00	1.329	1.343	1.342	1.343
					230.00	1.395	1.388	1.387	1.388
					240.00	1.460	1.433	1.432	1.433
					250.00	1.536	1.478	1.477	1.478
Tritriacontane	C33H68	352.686	0.217	Test set 1, Training set 2	93.70	0.703	0.721	0.720	0.721
					122.20	0.841	0.876	0.875	0.876
					146.00	0.950	0.996	0.995	0.996
					163.30	1.038	1.079	1.078	1.079
					165.00	1.042	1.087	1.086	1.087
					184.00	1.138	1.176	1.175	1.176

					207.00	1.268	1.283	1.282	1.283
					227.30	1.385	1.375	1.374	1.375
					252.00	1.540	1.487	1.486	1.487

Alkenes									
1-Decene	C10H20	140.27	0.214	Test set 1, Training set 2	50.00	0.440	0.399	0.428	0.399
					60.00	0.538	0.484	0.520	0.484
					70.00	0.624	0.559	0.600	0.559
					80.00	0.700	0.626	0.670	0.626
					90.00	0.771	0.687	0.734	0.687
					100.00	0.832	0.744	0.793	0.744
					110.00	0.890	0.799	0.849	0.799
					120.00	0.946	0.851	0.903	0.851
					130.00	0.999	0.902	0.955	0.902
					140.00	1.053	0.951	1.005	0.951
					150.00	1.106	1.000	1.054	1.000
					160.00	1.161	1.048	1.103	1.048
					170.00	1.219	1.095	1.150	1.095
					180.00	1.286	1.142	1.197	1.142

					190.00	1.360	1.188	1.244	1.188
1-Undecene	C11H22	154.29	0.214	Test set 1, Training set 2	50.00	0.431	0.399	0.428	0.399
					60.00	0.530	0.484	0.520	0.484
					70.00	0.616	0.559	0.600	0.559
					80.00	0.692	0.626	0.670	0.626
					90.00	0.762	0.687	0.734	0.687
					100.00	0.820	0.744	0.793	0.744
					110.00	0.877	0.799	0.849	0.799
					120.00	0.931	0.851	0.903	0.851
					130.00	0.982	0.902	0.955	0.902
					140.00	1.033	0.951	1.005	0.951
					150.00	1.084	1.000	1.054	1.000
					160.00	1.136	1.048	1.103	1.048
					170.00	1.190	1.095	1.150	1.095
					180.00	1.247	1.142	1.197	1.142
					190.00	1.308	1.188	1.244	1.188
					200.00	1.377	1.234	1.290	1.234
					210.00	1.460	1.280	1.336	1.280
1-Dodecene	C12H24	168.32	0.214	Test set 1, Training	50.00	0.432	0.399	0.428	0.399

				set 2	60.00	0.529	0.484	0.520	0.484
					70.00	0.615	0.559	0.600	0.559
					80.00	0.693	0.626	0.670	0.626
					90.00	0.764	0.687	0.734	0.687
					100.00	0.826	0.744	0.793	0.744
					110.00	0.884	0.799	0.849	0.799
					120.00	0.941	0.851	0.903	0.851
					130.00	0.995	0.902	0.955	0.902
					140.00	1.048	0.951	1.005	0.951
					150.00	1.104	1.000	1.054	1.000
					160.00	1.162	1.048	1.103	1.048
					170.00	1.225	1.095	1.150	1.095
					180.00	1.296	1.142	1.197	1.142
					190.00	1.380	1.188	1.244	1.188
1-Hexadecene	C16H32	224.43	0.214	Training set 1, Training set 2	50.00	0.403	0.399	0.428	0.399
					60.00	0.501	0.484	0.52	0.484
					70.00	0.586	0.559	0.5996	0.559
					80.00	0.660	0.626	0.67	0.626
					90.00	0.728	0.687	0.7339	0.687

					100.00	0.789	0.744	0.7933	0.744
					110.00	0.847	0.799	0.8493	0.799
					120.00	0.903	0.851	0.9028	0.851
					130.00	0.956	0.902	0.9545	0.902
					140.00	1.008	0.951	1.0048	0.951
					150.00	1.055	1.000	1.054	1.000
					160.00	1.107	1.048	1.1024	1.048
					170.00	1.161	1.095	1.1501	1.095
					180.00	1.218	1.142	1.1972	1.142
					185.00	1.249	1.165	1.2206	1.165
					190.00	1.284	1.188	1.2439	1.188
					195.00	1.318	1.211	1.2671	1.211

Alcohols									
					50.00	0.387	0.385	0.375	0.424
					60.00	0.484	0.467	0.456	0.506
					70.00	0.572	0.539	0.526	0.578
					80.00	0.651	0.604	0.590	0.643
					90.00	0.722	0.664	0.648	0.703

1- Octanol	C8H18O	130.23	0.207	Test set 1, Training set 2	100.00	0.784	0.720	0.704	0.759
					110.00	0.842	0.773	0.756	0.812
					120.00	0.895	0.824	0.807	0.863
					130.00	0.944	0.874	0.857	0.913
					140.00	0.991	0.922	0.905	0.962
					150.00	1.037	0.970	0.952	1.009
					160.00	1.084	1.017	0.999	1.056
					170.00	1.129	1.064	1.046	1.103
					180.00	1.174	1.110	1.092	1.149
					190.00	1.219	1.156	1.138	1.195
					200.00	1.268	1.202	1.183	1.241
					210.00	1.318	1.247	1.228	1.286
					220.00	1.368	1.292	1.273	1.331
					230.00	1.417	1.337	1.318	1.376
					240.00	1.467	1.382	1.363	1.421
					250.00	1.517	1.426	1.408	1.465
					258.43	1.560	1.464	1.445	1.503
					50.00	0.369	0.387	0.378	0.420
					60.00	0.469	0.470	0.458	0.502

1-Decanol	C10H22O	158.28	0.208	Test set 1, Training set 2	70.00	0.556	0.543	0.529	0.575
					80.00	0.634	0.608	0.593	0.640
					90.00	0.705	0.668	0.652	0.700
					100.00	0.765	0.724	0.708	0.756
					110.00	0.816	0.777	0.761	0.810
					120.00	0.868	0.829	0.812	0.861
					130.00	0.915	0.879	0.861	0.911
					140.00	0.969	0.928	0.910	0.960
					150.00	1.009	0.976	0.958	1.008
					160.00	1.054	1.023	1.005	1.055
					170.00	1.096	1.070	1.051	1.102
					180.00	1.138	1.116	1.097	1.148
					190.00	1.180	1.162	1.143	1.194
					200.00	1.224	1.207	1.189	1.239
					210.00	1.274	1.253	1.234	1.285
					220.00	1.331	1.298	1.279	1.330
					230.00	1.386	1.343	1.324	1.375
					240.00	1.443	1.388	1.369	1.420
					250.00	1.499	1.432	1.413	1.465

					260.00	1.556	1.477	1.458	1.509
					270.00	1.612	1.521	1.502	1.554
					280.00	1.669	1.566	1.547	1.598
1-Dodecanol	C12H26O	186.33	0.209	Test set 1, Training set 2	50.00	0.377	0.389	0.380	0.416
					60.00	0.469	0.472	0.460	0.500
					70.00	0.552	0.545	0.532	0.573
					80.00	0.625	0.611	0.596	0.638
					90.00	0.691	0.671	0.655	0.698
					100.00	0.749	0.727	0.711	0.754
					110.00	0.804	0.781	0.764	0.808
					120.00	0.854	0.832	0.815	0.859
					130.00	0.901	0.882	0.865	0.910
					140.00	0.945	0.931	0.913	0.958
					150.00	0.989	0.979	0.961	1.006
					160.00	1.033	1.027	1.008	1.054
					170.00	1.074	1.073	1.055	1.101
					180.00	1.118	1.120	1.101	1.147
					190.00	1.163	1.166	1.147	1.193
					200.00	1.210	1.211	1.193	1.239

					210.00	1.259	1.257	1.238	1.284
					220.00	1.311	1.302	1.283	1.329
					230.00	1.367	1.347	1.328	1.374
					240.00	1.427	1.392	1.373	1.419
					250.00	1.494	1.437	1.417	1.464
					260.00	1.567	1.481	1.462	1.509
1-Tridecal	C13H28O	200.365	0.210	Test set 1, Training set 2	50.00	0.371	0.390	0.380	0.415
					60.00	0.464	0.473	0.461	0.499
					70.00	0.547	0.546	0.533	0.572
					80.00	0.620	0.612	0.597	0.637
					90.00	0.685	0.672	0.656	0.697
					100.00	0.743	0.728	0.712	0.754
					110.00	0.799	0.782	0.765	0.807
					120.00	0.848	0.834	0.816	0.859
					130.00	0.895	0.884	0.866	0.909
					140.00	0.939	0.933	0.915	0.958
					150.00	0.982	0.981	0.962	1.006
					160.00	1.026	1.028	1.010	1.053
					170.00	1.067	1.075	1.056	1.100

					180.00	1.109	1.121	1.103	1.147
					190.00	1.155	1.167	1.148	1.193
					200.00	1.201	1.213	1.194	1.238
					210.00	1.251	1.258	1.239	1.284
					220.00	1.303	1.304	1.285	1.329
					230.00	1.355	1.349	1.330	1.374
					240.00	1.416	1.394	1.374	1.419
					250.00	1.482	1.438	1.419	1.464
					260.00	1.555	1.483	1.464	1.508
1-Octdecanol	C18H38O	270.4991	0.211	Training set 1, Training set 2	50.00	0.364	0.392	0.383	0.411
					55.00	0.412	0.436	0.425	0.455
					60.00	0.457	0.476	0.464	0.495
					65.00	0.499	0.514	0.501	0.533
					70.00	0.539	0.550	0.536	0.568
					75.00	0.577	0.583	0.569	0.602
					80.00	0.612	0.615	0.601	0.634
					85.00	0.645	0.646	0.631	0.665
					90.00	0.677	0.676	0.660	0.695
					95.00	0.707	0.705	0.688	0.723

					100.00	0.733	0.732	0.716	0.751
					105.00	0.761	0.760	0.743	0.778
					110.00	0.787	0.786	0.769	0.805
					120.00	0.836	0.838	0.821	0.857
					130.00	0.882	0.888	0.870	0.907
					140.00	0.925	0.937	0.919	0.956
					150.00	0.968	0.986	0.967	1.004
					160.00	1.010	1.033	1.015	1.052
					170.00	1.052	1.080	1.061	1.099
					180.00	1.094	1.127	1.108	1.145
					190.00	1.138	1.173	1.154	1.191
					200.00	1.183	1.218	1.199	1.237
					210.00	1.230	1.264	1.245	1.283
					220.00	1.278	1.309	1.290	1.328
					230.00	1.329	1.354	1.335	1.373
					240.00	1.383	1.399	1.380	1.418
					250.00	1.440	1.444	1.425	1.463
					260.00	1.498	1.489	1.469	1.508
1-Nonadecanol	C19H40O	284.526	0.211	Training set 1,	50.00	0.357	0.393	0.383	0.411

				Training set 2	55.00	0.406	0.436	0.425	0.454
					60.00	0.451	0.477	0.465	0.494
					65.00	0.493	0.514	0.502	0.532
					70.00	0.532	0.550	0.536	0.568
					75.00	0.570	0.584	0.569	0.602
					80.00	0.604	0.616	0.601	0.634
					85.00	0.637	0.647	0.631	0.665
					90.00	0.670	0.676	0.661	0.694
					95.00	0.698	0.705	0.689	0.723
					100.00	0.725	0.733	0.717	0.751
					105.00	0.755	0.760	0.743	0.778
					110.00	0.780	0.787	0.770	0.805
					120.00	0.829	0.839	0.821	0.857
					130.00	0.875	0.889	0.871	0.907
					140.00	0.918	0.938	0.920	0.956
					150.00	0.961	0.986	0.968	1.004
					160.00	1.002	1.034	1.015	1.052
					170.00	1.044	1.081	1.062	1.099
					180.00	1.085	1.127	1.108	1.145

					190.00	1.129	1.173	1.154	1.191
					200.00	1.173	1.219	1.200	1.237
					210.00	1.220	1.265	1.246	1.283
					220.00	1.269	1.310	1.291	1.328
					230.00	1.320	1.355	1.336	1.373
					240.00	1.374	1.400	1.381	1.418
					250.00	1.431	1.445	1.425	1.463
					260.00	1.487	1.490	1.470	1.507
1-Eicosanol	C20H42O	298.55	0.211	Test set 1, Training set 2	50.00	0.359	0.393	0.383	0.410
					55.00	0.408	0.436	0.425	0.453
					60.00	0.453	0.477	0.465	0.494
					65.00	0.494	0.515	0.502	0.532
					70.00	0.534	0.551	0.537	0.568
					75.00	0.571	0.584	0.570	0.601
					80.00	0.604	0.616	0.601	0.633
					85.00	0.640	0.647	0.632	0.664
					90.00	0.671	0.677	0.661	0.694
					95.00	0.700	0.706	0.689	0.723
					100.00	0.730	0.734	0.717	0.751

					105.00	0.757	0.761	0.744	0.778
					110.00	0.783	0.787	0.770	0.804
					120.00	0.831	0.839	0.822	0.856
					130.00	0.877	0.890	0.872	0.907
					140.00	0.920	0.939	0.920	0.956
					150.00	0.963	0.987	0.968	1.004
					160.00	1.007	1.034	1.016	1.051
					170.00	1.047	1.081	1.063	1.098
					180.00	1.089	1.128	1.109	1.145
					190.00	1.133	1.174	1.155	1.191
					200.00	1.179	1.220	1.201	1.237
					210.00	1.227	1.265	1.246	1.282
					220.00	1.275	1.311	1.291	1.328
					230.00	1.326	1.356	1.336	1.373
					240.00	1.381	1.401	1.381	1.418
					250.00	1.439	1.446	1.426	1.463
					260.00	1.499	1.490	1.471	1.507
					270.00	1.567	1.535	1.515	1.552
					280.00	1.644	1.579	1.560	1.596

1-Docosanol	C22H46O	326.61	0.211	Test set 1, Training set 2	50.00	0.354	0.393	0.384	0.409
					55.00	0.401	0.437	0.426	0.453
					60.00	0.445	0.478	0.465	0.493
					65.00	0.489	0.516	0.502	0.531
					70.00	0.528	0.551	0.537	0.567
					75.00	0.567	0.585	0.571	0.601
					80.00	0.602	0.617	0.602	0.633
					85.00	0.634	0.648	0.633	0.664
					90.00	0.666	0.678	0.662	0.693
					95.00	0.695	0.707	0.690	0.722
					100.00	0.725	0.735	0.718	0.750
					105.00	0.751	0.762	0.745	0.777
					110.00	0.777	0.788	0.771	0.804
					120.00	0.825	0.840	0.823	0.856
					130.00	0.871	0.891	0.873	0.906
					140.00	0.914	0.940	0.921	0.955
					150.00	0.956	0.988	0.969	1.004
					160.00	0.998	1.036	1.017	1.051
					170.00	1.040	1.083	1.064	1.098

					180.00	1.082	1.129	1.110	1.145
					190.00	1.125	1.175	1.156	1.191
					200.00	1.171	1.221	1.202	1.237
					210.00	1.216	1.267	1.247	1.282
					220.00	1.264	1.312	1.293	1.328
					230.00	1.314	1.357	1.338	1.373
					240.00	1.366	1.402	1.383	1.418
					250.00	1.421	1.447	1.427	1.462
					260.00	1.480	1.492	1.472	1.507
					270.00	1.541	1.536	1.516	1.552
					280.00	1.610	1.581	1.561	1.596
					290.00	1.685	1.625	1.605	1.640
					298.15	1.753	1.661	1.641	1.676
					300.00	1.775	1.669	1.649	1.685
					310.00	1.876	1.713	1.693	1.729
					343.92	2.085	1.862	1.843	1.878

Esters									
Methyl Octanoate	C9H18O2	158.24	0.183	Test set 1, Training	50.00	0.419	0.334	0.360	0.398

				set 2	60.00	0.504	0.405	0.437	0.469
					70.00	0.583	0.468	0.505	0.533
					80.00	0.653	0.526	0.566	0.590
					90.00	0.717	0.579	0.622	0.644
					100.00	0.773	0.630	0.674	0.694
					110.00	0.828	0.678	0.724	0.743
					120.00	0.877	0.725	0.773	0.790
					130.00	0.924	0.771	0.819	0.836
					140.00	0.970	0.817	0.865	0.881
					150.00	1.013	0.861	0.911	0.925
					160.00	1.056	0.905	0.955	0.970
					170.00	1.101	0.949	1.000	1.014
					180.00	1.146	0.993	1.044	1.057
					190.00	1.193	1.036	1.087	1.101
					200.00	1.245	1.080	1.131	1.144
					210.00	1.302	1.123	1.174	1.187
					220.00	1.376	1.166	1.218	1.230
Methyl Nonanoate	C10H20O2	172.27	0.186	Test set 1, Training set 2	50.00	0.414	0.339	0.366	0.398
					60.00	0.502	0.411	0.445	0.470

					70.00	0.584	0.476	0.513	0.534
					80.00	0.656	0.534	0.575	0.593
					90.00	0.720	0.588	0.632	0.647
					100.00	0.780	0.639	0.685	0.698
					110.00	0.835	0.688	0.735	0.747
					120.00	0.884	0.736	0.784	0.794
					130.00	0.932	0.782	0.831	0.841
					140.00	0.978	0.828	0.878	0.886
					150.00	1.021	0.873	0.923	0.931
					160.00	1.064	0.917	0.968	0.976
					170.00	1.108	0.961	1.013	1.020
					180.00	1.152	1.005	1.057	1.064
					190.00	1.199	1.049	1.101	1.108
					200.00	1.250	1.093	1.145	1.151
					210.00	1.304	1.136	1.189	1.195
					220.00	1.373	1.180	1.232	1.238
Methyl Decanoate	C11H22O2	186.29	0.188	Test set 1, Training set 2	50.00	0.406	0.343	0.371	0.398
					60.00	0.491	0.417	0.451	0.471
					70.00	0.569	0.482	0.520	0.536

					80.00	0.639	0.541	0.583	0.595
					90.00	0.704	0.595	0.640	0.650
					100.00	0.760	0.647	0.693	0.702
					110.00	0.814	0.696	0.744	0.751
					120.00	0.862	0.744	0.794	0.799
					130.00	0.908	0.791	0.841	0.846
					140.00	0.952	0.837	0.888	0.891
					150.00	0.994	0.882	0.934	0.937
					160.00	1.036	0.927	0.979	0.982
					170.00	1.078	0.971	1.024	1.026
					180.00	1.122	1.016	1.069	1.070
					190.00	1.167	1.060	1.113	1.114
					200.00	1.215	1.103	1.157	1.158
					210.00	1.261	1.147	1.201	1.202
					220.00	1.315	1.191	1.245	1.245
					230.00	1.374	1.234	1.289	1.289
Methyl Undecanoate	C12H24O2	200.32	0.190	Test set 1, Training set 2	50.00	0.400	0.347	0.375	0.398
					60.00	0.489	0.421	0.456	0.472
					70.00	0.568	0.487	0.526	0.538

					80.00	0.639	0.547	0.589	0.597
					90.00	0.706	0.602	0.647	0.652
					100.00	0.763	0.654	0.701	0.704
					110.00	0.818	0.703	0.752	0.754
					120.00	0.866	0.752	0.802	0.802
					130.00	0.913	0.799	0.850	0.849
					140.00	0.957	0.845	0.897	0.896
					150.00	1.001	0.890	0.943	0.941
					160.00	1.045	0.935	0.989	0.986
					170.00	1.087	0.980	1.034	1.031
					180.00	1.131	1.025	1.078	1.075
					190.00	1.175	1.069	1.123	1.119
					200.00	1.221	1.113	1.167	1.163
					210.00	1.268	1.157	1.211	1.207
					220.00	1.323	1.200	1.255	1.251
					230.00	1.383	1.244	1.299	1.295
Methyl Dodecanoate	C13H26O2	214.35	0.191	Test set 1, Training set 2	50.00	0.397	0.351	0.379	0.398
					60.00	0.481	0.426	0.460	0.473
					70.00	0.555	0.492	0.532	0.539

					80.00	0.628	0.552	0.595	0.599
					90.00	0.694	0.607	0.653	0.655
					100.00	0.749	0.660	0.708	0.707
					110.00	0.802	0.710	0.759	0.757
					120.00	0.849	0.758	0.809	0.806
					130.00	0.895	0.805	0.857	0.853
					140.00	0.938	0.852	0.905	0.899
					150.00	0.979	0.898	0.951	0.945
					160.00	1.021	0.943	0.997	0.990
					170.00	1.064	0.988	1.042	1.035
					180.00	1.107	1.032	1.087	1.080
					190.00	1.151	1.077	1.132	1.124
					200.00	1.195	1.121	1.176	1.168
					210.00	1.240	1.165	1.220	1.212
					220.00	1.293	1.209	1.265	1.256
					230.00	1.346	1.253	1.309	1.300
					240.00	1.399	1.296	1.353	1.344
Ethyl Undecanoate	C13H26O2	214.34	0.191	Training set 1, Training set 2	111.58	0.810	0.717	0.767	0.765
					113.84	0.821	0.728	0.779	0.776

					116.71	0.835	0.742	0.793	0.790
					119.57	0.849	0.756	0.807	0.804
					122.42	0 .864	0.770	0.821	0.817
					125.29	0.877	0.783	0.835	0.831
					128.15	0.889	0.797	0.849	0.844
					131.02	0.907	0.810	0.862	0.858
					133.86	0.927	0.823	0.876	0.871
					136.66	0.926	0.836	0.889	0.884
					139.44	0.941	0.849	0.902	0.897
					142.19	0.955	0.862	0.915	0.909
					144.90	0.970	0.874	0.927	0.922
					147.59	0.986	0.887	0.940	0.934
					150.26	0.997	0.899	0.952	0.946
					152.89	1.014	0.911	0.964	0.958
					155.51	1.031	0.923	0.976	0.970
					158.10	1.045	0.934	0.988	0.982
					160.67	1.069	0.946	1.000	0.993
					163.21	1.088	0.957	1.011	1.005
					165.73	1.102	0.969	1.023	1.016

					168.24	1.076	0.980	1.034	1.027
					170.74	1.083	0.991	1.046	1.038
					173.23	1.095	1.002	1.057	1.050
					175.70	1.105	1.013	1.068	1.061
					178.15	1.117	1.024	1.079	1.072
					180.59	1.130	1.035	1.090	1.082
					183.01	1.139	1.046	1.101	1.093
					185.42	1.147	1.056	1.111	1.104
					187.81	1.158	1.067	1.122	1.114
					190.18	1.175	1.077	1.133	1.125
					192.55	1.196	1.088	1.143	1.135
					194.90	1.200	1.098	1.154	1.146
					197.24	1.203	1.109	1.164	1.156
					199.56	1.223	1.119	1.174	1.166
					201.88	1.243	1.129	1.185	1.177
					204.18	1.259	1.139	1.195	1.187
					206.47	1.252	1.149	1.205	1.197
					208.75	1.270	1.159	1.215	1.207
					211.01	1.288	1.169	1.225	1.217

					213.26	1.304	1.179	1.235	1.227
					215.50	1.304	1.189	1.245	1.236
					217.73	1.323	1.199	1.255	1.246
					219.95	1.341	1.209	1.264	1.256
Methyl tridecanoate	C14H28O2	228.37	0.193	Test set 1, Training set 2	50.00	0.390	0.354	0.382	0.398
					60.00	0.476	0.429	0.464	0.474
					70.00	0.560	0.496	0.536	0.540
					80.00	0.633	0.556	0.600	0.601
					90.00	0.696	0.612	0.659	0.657
					100.00	0.752	0.665	0.713	0.709
					110.00	0.805	0.715	0.765	0.760
					120.00	0.855	0.764	0.815	0.808
					130.00	0.900	0.811	0.864	0.856
					140.00	0.944	0.858	0.911	0.903
					150.00	0.987	0.904	0.958	0.948
					160.00	1.029	0.949	1.004	0.994
					170.00	1.071	0.994	1.049	1.039
					180.00	1.113	1.039	1.095	1.084
					190.00	1.156	1.084	1.139	1.128

					200.00	1.201	1.128	1.184	1.172
					210.00	1.247	1.172	1.228	1.217
					220.00	1.296	1.216	1.273	1.261
					230.00	1.348	1.260	1.317	1.305
					240.00	1.406	1.304	1.361	1.348
					250.00	1.472	1.348	1.405	1.392
Methyl Tetradecanoate	C15H30O2	242.4	0.194	Test set 1, Training set 2	50.00	0.386	0.356	0.385	0.398
					60.00	0.470	0.432	0.468	0.474
					70.00	0.550	0.499	0.540	0.541
					80.00	0.620	0.560	0.605	0.602
					90.00	0.683	0.616	0.664	0.658
					100.00	0.740	0.669	0.719	0.711
					110.00	0.792	0.720	0.771	0.762
					120.00	0.840	0.769	0.821	0.811
					130.00	0.885	0.817	0.870	0.859
					140.00	0.928	0.863	0.917	0.905
					150.00	0.970	0.910	0.964	0.951
					160.00	1.010	0.955	1.010	0.997
					170.00	1.052	1.000	1.056	1.042

					180.00	1.094	1.045	1.101	1.087
					190.00	1.137	1.090	1.146	1.132
					200.00	1.180	1.134	1.191	1.176
					210.00	1.224	1.178	1.235	1.220
					220.00	1.274	1.223	1.280	1.264
					230.00	1.324	1.267	1.324	1.309
					240.00	1.380	1.311	1.368	1.353
					250.00	1.442	1.355	1.412	1.396
Ethyl Tridecanoate	C15H30O2	242.4	0.194	Training set 1, Training set 2	203.72	1.251	1.151	1.207	1.193
					204.30	1.256	1.153	1.210	1.195
					206.07	1.266	1.161	1.218	1.203
					209.03	1.282	1.174	1.231	1.216
					211.98	1.296	1.187	1.244	1.229
					214.92	1.312	1.200	1.257	1.242
					217.87	1.328	1.213	1.270	1.255
					220.82	1.344	1.226	1.283	1.268
					223.77	1.360	1.239	1.296	1.281
					226.72	1.378	1.252	1.310	1.294
					229.65	1.396	1.265	1.323	1.307

					232.57	1.414	1.278	1.335	1.320
					235.47	1.433	1.291	1.348	1.333
					238.34	1.454	1.303	1.361	1.345
					241.19	1.474	1.316	1.373	1.358
					244.03	1.495	1.328	1.386	1.370
Methyl Pentadecanoate	C16H32O2	256.43	0.195	Test set 1, Training set 2	50.00	0.381	0.358	0.388	0.399
					60.00	0.469	0.435	0.471	0.475
					70.00	0.551	0.503	0.544	0.543
					80.00	0.621	0.564	0.609	0.604
					90.00	0.686	0.620	0.668	0.660
					100.00	0.742	0.673	0.723	0.714
					110.00	0.795	0.724	0.776	0.764
					120.00	0.844	0.773	0.826	0.813
					130.00	0.889	0.821	0.875	0.861
					140.00	0.933	0.868	0.923	0.908
					150.00	0.975	0.914	0.970	0.955
					160.00	1.016	0.960	1.016	1.000
					170.00	1.062	1.005	1.062	1.046
					180.00	1.100	1.050	1.107	1.091

					190.00	1.143	1.095	1.152	1.135
					200.00	1.187	1.140	1.197	1.180
					210.00	1.233	1.184	1.242	1.224
					220.00	1.282	1.228	1.286	1.268
					230.00	1.333	1.272	1.330	1.313
					240.00	1.388	1.316	1.375	1.357
					250.00	1.448	1.360	1.419	1.401
Methyl Hexanoate	C17H34O2	270.45	0.196	Test set 1, Training set 2	50.00	0.385	0.361	0.390	0.398
					60.00	0.480	0.438	0.474	0.475
					70.00	0.559	0.506	0.547	0.543
					80.00	0.618	0.567	0.612	0.605
					90.00	0.681	0.624	0.672	0.661
					100.00	0.733	0.677	0.727	0.715
					110.00	0.789	0.728	0.780	0.766
					120.00	0.837	0.777	0.831	0.815
					130.00	0.882	0.825	0.880	0.863
					140.00	0.925	0.873	0.928	0.910
					150.00	0.967	0.919	0.975	0.956
					160.00	1.008	0.965	1.021	1.002

					170.00	1.050	1.010	1.067	1.048
					180.00	1.092	1.055	1.112	1.093
					190.00	1.134	1.100	1.157	1.138
					200.00	1.178	1.145	1.202	1.182
					210.00	1.224	1.189	1.247	1.227
					220.00	1.272	1.233	1.292	1.271
					230.00	1.323	1.278	1.336	1.315
					240.00	1.377	1.322	1.380	1.359
					250.00	1.436	1.366	1.425	1.403
Methyl Heptadecanoate	C18H36O2	284.48	0.197	Test set 1, Training set 2	50.00	0.376	0.362	0.392	0.398
					60.00	0.463	0.440	0.477	0.476
					70.00	0.544	0.508	0.550	0.544
					80.00	0.617	0.570	0.615	0.606
					90.00	0.678	0.627	0.675	0.663
					100.00	0.733	0.680	0.731	0.716
					110.00	0.788	0.732	0.784	0.767
					120.00	0.838	0.781	0.835	0.817
					130.00	0.888	0.829	0.884	0.865
					140.00	0.934	0.876	0.932	0.912

					150.00	0.969	0.923	0.979	0.959
					160.00	1.000	0.969	1.026	1.005
					170.00	1.062	1.014	1.072	1.050
					180.00	1.103	1.060	1.117	1.095
					190.00	1.147	1.104	1.162	1.140
					200.00	1.195	1.149	1.207	1.185
					210.00	1.250	1.194	1.252	1.229
					220.00	1.293	1.238	1.297	1.274
					230.00	1.346	1.282	1.341	1.318
					240.00	1.404	1.326	1.386	1.362
					250.00	1.471	1.371	1.430	1.406
Methy Octadecanoate	C19H38O2	298.5	0.198	Test set 1, Training set 2	50.00	0.376	0.364	0.394	0.398
					60.00	0.462	0.442	0.479	0.476
					70.00	0.545	0.511	0.553	0.545
					80.00	0.613	0.572	0.618	0.607
					90.00	0.675	0.630	0.678	0.664
					100.00	0.728	0.683	0.734	0.717
					110.00	0.784	0.735	0.787	0.769
					120.00	0.831	0.784	0.838	0.818

					130.00	0.877	0.833	0.888	0.867
					140.00	0.920	0.880	0.936	0.914
					150.00	0.961	0.927	0.983	0.961
					160.00	1.003	0.973	1.030	1.007
					170.00	1.048	1.018	1.076	1.052
					180.00	1.096	1.063	1.121	1.097
					190.00	1.145	1.108	1.167	1.142
					200.00	1.188	1.153	1.212	1.187
					210.00	1.233	1.198	1.257	1.232
					220.00	1.282	1.242	1.301	1.276
					230.00	1.333	1.286	1.346	1.321
					240.00	1.384	1.331	1.390	1.365
					250.00	1.436	1.375	1.435	1.409
Methyl Nonadecanoate	C20H40O2	312.53	0.198	Test set 1, Training set 2	50.00	0.377	0.366	0.396	0.398
					60.00	0.460	0.444	0.481	0.476
					70.00	0.541	0.513	0.555	0.545
					80.00	0.610	0.575	0.621	0.607
					90.00	0.673	0.632	0.681	0.665
					100.00	0.732	0.686	0.737	0.719

					110.00	0.782	0.738	0.791	0.770
					120.00	0.829	0.787	0.842	0.820
					130.00	0.874	0.836	0.891	0.868
					140.00	0.918	0.883	0.939	0.916
					150.00	0.960	0.930	0.987	0.962
					160.00	1.003	0.976	1.033	1.008
					170.00	1.047	1.022	1.080	1.054
					180.00	1.086	1.067	1.125	1.099
					190.00	1.130	1.112	1.171	1.145
					200.00	1.175	1.157	1.216	1.189
					210.00	1.219	1.201	1.261	1.234
					220.00	1.272	1.246	1.305	1.278
					230.00	1.324	1.290	1.350	1.323
					240.00	1.383	1.335	1.395	1.367
					250.00	1.442	1.379	1.439	1.411
Methyl Eicosanoate	C21H42O2	326.56	0.199	Test set 1, Training set 2	50.00	0.375	0.367	0.398	0.398
					60.00	0.459	0.446	0.483	0.477
					70.00	0.541	0.515	0.557	0.546
					80.00	0.612	0.577	0.624	0.608

					90.00	0.674	0.635	0.684	0.666
					100.00	0.722	0.689	0.740	0.720
					110.00	0.781	0.740	0.793	0.771
					120.00	0.830	0.790	0.845	0.821
					130.00	0.874	0.839	0.894	0.870
					140.00	0.917	0.886	0.943	0.917
					150.00	0.959	0.933	0.990	0.964
					160.00	1.000	0.979	1.037	1.010
					170.00	1.041	1.025	1.083	1.056
					180.00	1.082	1.070	1.129	1.101
					190.00	1.124	1.115	1.174	1.146
					200.00	1.167	1.160	1.220	1.191
					210.00	1.212	1.205	1.265	1.236
					220.00	1.259	1.249	1.309	1.281
					230.00	1.308	1.294	1.354	1.325
					240.00	1.359	1.338	1.398	1.369
					250.00	1.413	1.382	1.443	1.414

Carboxylic Acid

Heptanoic Acid	C7H14O2	130.19	0.177	Test set 1, Training set 2	105.00	0.774	0.629	0.649	0.707
					110.00	0.796	0.653	0.673	0.731
					115.00	0.821	0.676	0.696	0.754
					120.00	0.843	0.699	0.719	0.777
					125.00	0.866	0.721	0.742	0.799
					130.00	0.889	0.743	0.765	0.821
					135.00	0.913	0.766	0.787	0.844
					140.00	0.935	0.788	0.809	0.866
					145.00	0.957	0.809	0.831	0.887
					150.00	0.979	0.831	0.853	0.909
					155.00	1.003	0.853	0.875	0.931
					160.00	1.026	0.874	0.897	0.952
					165.00	1.049	0.896	0.918	0.974
					170.00	1.072	0.917	0.940	0.996
					175.00	1.096	0.939	0.961	1.017
					180.00	1.123	0.960	0.983	1.038
					185.00	1.151	0.982	1.004	1.060
					190.00	1.179	1.003	1.026	1.081
					195.00	1.214	1.024	1.047	1.102

					200.00	1.252	1.046	1.068	1.124
					205.00	1.295	1.067	1.090	1.145
					210.00	1.341	1.088	1.111	1.166
					215.00	1.389	1.109	1.132	1.187
					220.00	1.444	1.131	1.154	1.209
Octanoic Acid	C8H16O2	144.21	0.180	Test set 1, Training set 2	155.00	1.012	0.870	0.892	0.940
					160.00	1.036	0.891	0.914	0.962
					165.00	1.060	0.913	0.936	0.984
					170.00	1.085	0.935	0.958	1.005
					175.00	1.111	0.957	0.980	1.027
					180.00	1.136	0.978	1.002	1.049
					185.00	1.165	1.000	1.023	1.070
					190.00	1.194	1.021	1.045	1.092
					195.00	1.225	1.043	1.066	1.113
					200.00	1.256	1.064	1.088	1.135
					205.00	1.288	1.086	1.109	1.156
					210.00	1.321	1.107	1.131	1.178
					215.00	1.356	1.129	1.152	1.199
					220.00	1.392	1.150	1.174	1.221

					225.00	1.436	1.172	1.195	1.242
					230.00	1.468	1.193	1.217	1.264
					235.00	1.512	1.215	1.238	1.285
					240.00	1.554	1.236	1.260	1.306
					245.00	1.593	1.257	1.281	1.328
					250.00	1.630	1.279	1.303	1.349
					255.00	1.678	1.300	1.324	1.371
					260.00	1.727	1.322	1.346	1.392
Nonanoic Acid	C9H18O2	158.24	0.183	Test set 1, Training set 2	90.00	0.679	0.579	0.600	0.644
					95.00	0.706	0.605	0.626	0.669
					100.00	0.732	0.630	0.651	0.694
					105.00	0.757	0.654	0.676	0.719
					110.00	0.782	0.678	0.700	0.743
					115.00	0.805	0.702	0.724	0.766
					120.00	0.828	0.725	0.748	0.790
					125.00	0.852	0.749	0.771	0.813
					130.00	0.873	0.771	0.794	0.836
					135.00	0.896	0.794	0.817	0.858
					140.00	0.917	0.817	0.840	0.881

					145.00	0.939	0.839	0.862	0.903
					150.00	0.959	0.861	0.885	0.925
					155.00	0.980	0.883	0.907	0.948
					160.00	1.001	0.905	0.929	0.970
					165.00	1.023	0.927	0.951	0.992
					170.00	1.048	0.949	0.973	1.014
					175.00	1.068	0.971	0.995	1.035
					180.00	1.091	0.993	1.017	1.057
					185.00	1.114	1.015	1.039	1.079
					190.00	1.138	1.036	1.061	1.101
					195.00	1.163	1.058	1.082	1.122
					200.00	1.189	1.080	1.104	1.144
					205.00	1.217	1.101	1.126	1.166
					210.00	1.249	1.123	1.147	1.187
					215.00	1.285	1.145	1.169	1.209
Decanoic Acid	C10H20O2	172.268	0.186	Test set 1, Training set 2	90.00	0.683	0.588	0.609	0.647
					95.00	0.710	0.614	0.635	0.673
					100.00	0.736	0.639	0.661	0.698
					105.00	0.759	0.664	0.686	0.723

					110.00	0.782	0.688	0.710	0.747
					115.00	0.806	0.712	0.735	0.771
					120.00	0.830	0.736	0.759	0.795
					125.00	0.853	0.759	0.782	0.818
					130.00	0.875	0.782	0.805	0.841
					135.00	0.899	0.805	0.828	0.864
					140.00	0.919	0.828	0.851	0.887
					145.00	0.939	0.850	0.874	0.909
					150.00	0.961	0.873	0.897	0.932
					155.00	0.983	0.895	0.919	0.954
					160.00	1.004	0.917	0.941	0.976
					165.00	1.025	0.939	0.964	0.998
					170.00	1.049	0.961	0.986	1.020
					175.00	1.071	0.983	1.008	1.042
					180.00	1.094	1.005	1.030	1.064
					185.00	1.118	1.027	1.052	1.086
					190.00	1.141	1.049	1.074	1.108
					195.00	1.165	1.071	1.096	1.130
					200.00	1.193	1.093	1.117	1.152

					205.00	1.220	1.114	1.139	1.173
					210.00	1.248	1.136	1.161	1.195
					215.00	1.278	1.158	1.183	1.217
					220.00	1.309	1.180	1.205	1.239
					225.00	1.340	1.201	1.226	1.260
					230.00	1.370	1.223	1.248	1.282
Undecanoic Acid	C11H22O2	186.29	0.188	Test set 1, Training set 2	100.00	0.717	0.647	0.669	0.702
					105.00	0.741	0.672	0.694	0.726
					110.00	0.764	0.696	0.719	0.751
					115.00	0.788	0.720	0.744	0.775
					120.00	0.812	0.744	0.768	0.799
					125.00	0.835	0.768	0.791	0.822
					130.00	0.857	0.791	0.815	0.846
					135.00	0.880	0.814	0.838	0.869
					140.00	0.901	0.837	0.861	0.891
					145.00	0.921	0.860	0.884	0.914
					150.00	0.943	0.882	0.907	0.937
					155.00	0.966	0.905	0.929	0.959
					160.00	0.984	0.927	0.952	0.982

					165.00	1.006	0.949	0.974	1.004
					170.00	1.027	0.971	0.996	1.026
					175.00	1.049	0.994	1.019	1.048
					180.00	1.071	1.016	1.041	1.070
					185.00	1.096	1.038	1.063	1.092
					190.00	1.115	1.060	1.085	1.114
					195.00	1.137	1.082	1.107	1.136
					200.00	1.160	1.103	1.129	1.158
					205.00	1.183	1.125	1.151	1.180
					210.00	1.205	1.147	1.173	1.202
					215.00	1.230	1.169	1.195	1.224
					220.00	1.255	1.191	1.216	1.245
					225.00	1.278	1.213	1.238	1.267
					230.00	1.304	1.234	1.260	1.289
					235.00	1.331	1.256	1.282	1.311
Dodecaoinic Acid	C12H24O2	200.32	0.190	Test set 1, Training set 2	90.00	0.676	0.602	0.623	0.652
					95.00	0.702	0.628	0.650	0.679
					100.00	0.728	0.654	0.676	0.704
					105.00	0.751	0.679	0.702	0.730

					110.00	0.774	0.703	0.727	0.754
					115.00	0.799	0.728	0.751	0.779
					120.00	0.822	0.752	0.776	0.802
					125.00	0.844	0.775	0.799	0.826
					130.00	0.866	0.799	0.823	0.849
					135.00	0.888	0.822	0.846	0.873
					140.00	0.909	0.845	0.870	0.896
					145.00	0.930	0.868	0.893	0.919
					150.00	0.951	0.890	0.915	0.941
					155.00	0.972	0.913	0.938	0.964
					160.00	0.993	0.935	0.961	0.986
					165.00	1.014	0.958	0.983	1.009
					170.00	1.035	0.980	1.006	1.031
					175.00	1.056	1.002	1.028	1.053
					180.00	1.077	1.025	1.050	1.075
					185.00	1.101	1.047	1.072	1.097
					190.00	1.125	1.069	1.095	1.119
					195.00	1.147	1.091	1.117	1.142
					200.00	1.172	1.113	1.139	1.163

					205.00	1.196	1.135	1.161	1.185
					210.00	1.222	1.157	1.183	1.207
					215.00	1.246	1.179	1.205	1.229
					220.00	1.272	1.200	1.227	1.251
					225.00	1.302	1.222	1.248	1.273
					230.00	1.334	1.244	1.270	1.295
					235.00	1.365	1.266	1.292	1.317
					240.00	1.398	1.288	1.314	1.339
					245.00	1.431	1.310	1.336	1.360
					250.00	1.469	1.332	1.358	1.382
Tridecanoic Acid	C13H26O2	214.34824	0.191	Test set 1, Training set 2	90.00	0.661	0.607	0.629	0.655
					95.00	0.685	0.634	0.656	0.681
					100.00	0.712	0.660	0.682	0.707
					105.00	0.736	0.685	0.708	0.732
					110.00	0.760	0.710	0.733	0.757
					115.00	0.784	0.734	0.758	0.782
					120.00	0.807	0.758	0.782	0.806
					125.00	0.831	0.782	0.806	0.829
					130.00	0.852	0.805	0.830	0.853

					135.00	0.873	0.829	0.854	0.876
					140.00	0.894	0.852	0.877	0.899
					145.00	0.914	0.875	0.900	0.922
					150.00	0.936	0.898	0.923	0.945
					155.00	0.960	0.920	0.946	0.968
					160.00	0.979	0.943	0.968	0.990
					165.00	1.000	0.965	0.991	1.013
					170.00	1.021	0.988	1.014	1.035
					175.00	1.041	1.010	1.036	1.057
					180.00	1.061	1.032	1.058	1.080
					185.00	1.083	1.055	1.081	1.102
					190.00	1.105	1.077	1.103	1.124
					195.00	1.126	1.099	1.125	1.146
					200.00	1.148	1.121	1.147	1.168
					205.00	1.170	1.143	1.169	1.190
					210.00	1.190	1.165	1.191	1.212
					215.00	1.215	1.187	1.213	1.234
					220.00	1.239	1.209	1.235	1.256
					225.00	1.262	1.231	1.257	1.278

					230.00	1.287	1.253	1.279	1.300
					235.00	1.313	1.275	1.301	1.322
					240.00	1.340	1.296	1.323	1.344
					245.00	1.367	1.318	1.345	1.366
					250.00	1.395	1.340	1.367	1.388
					255.00	1.426	1.362	1.389	1.410
					260.00	1.457	1.384	1.411	1.431
					265.00	1.489	1.406	1.433	1.453
Tetradecanoic Acid	C14H28O2	228.37	0.193	Training set 1, Training set 2	90.00	0.669	0.612	0.634	0.657
					95.00	0.695	0.639	0.662	0.683
					100.00	0.721	0.665	0.688	0.709
					105.00	0.745	0.690	0.714	0.735
					110.00	0.769	0.715	0.739	0.760
					115.00	0.792	0.740	0.764	0.784
					120.00	0.814	0.764	0.789	0.808
					125.00	0.837	0.788	0.813	0.832
					130.00	0.860	0.811	0.837	0.856
					135.00	0.881	0.835	0.860	0.879
					140.00	0.903	0.858	0.884	0.903

					145.00	0.924	0.881	0.907	0.926
					150.00	0.945	0.904	0.930	0.948
					155.00	0.963	0.927	0.953	0.971
					160.00	0.984	0.949	0.976	0.994
					165.00	1.004	0.972	0.998	1.016
					170.00	1.024	0.994	1.021	1.039
					175.00	1.047	1.017	1.043	1.061
					180.00	1.068	1.039	1.066	1.084
					185.00	1.088	1.061	1.088	1.106
					190.00	1.110	1.084	1.110	1.128
					195.00	1.133	1.106	1.133	1.150
					200.00	1.157	1.128	1.155	1.172
					205.00	1.180	1.150	1.177	1.194
					210.00	1.204	1.172	1.199	1.217
					215.00	1.231	1.194	1.221	1.239
					220.00	1.257	1.216	1.243	1.261
					225.00	1.286	1.238	1.265	1.283
					230.00	1.315	1.260	1.287	1.305
					235.00	1.342	1.282	1.309	1.327

					240.00	1.372	1.304	1.331	1.348
Pentadecanoic Acid	C15H30O2	242.40	0.194	Training set 1, Training set 2	90.00	0.665	0.616	0.639	0.658
					95.00	0.692	0.643	0.666	0.685
					100.00	0.719	0.669	0.693	0.711
					105.00	0.743	0.695	0.719	0.737
					110.00	0.767	0.720	0.744	0.762
					115.00	0.790	0.745	0.769	0.787
					120.00	0.814	0.769	0.794	0.811
					125.00	0.836	0.793	0.818	0.835
					130.00	0.858	0.817	0.842	0.859
					135.00	0.880	0.840	0.866	0.882
					140.00	0.899	0.863	0.889	0.905
					145.00	0.921	0.887	0.913	0.928
					150.00	0.942	0.910	0.936	0.951
					155.00	0.962	0.932	0.959	0.974
					160.00	0.981	0.955	0.982	0.997
					165.00	1.002	0.978	1.004	1.020
					170.00	1.024	1.000	1.027	1.042
					175.00	1.046	1.023	1.050	1.065

					180.00	1.066	1.045	1.072	1.087
					185.00	1.088	1.067	1.094	1.109
					190.00	1.109	1.090	1.117	1.132
					195.00	1.131	1.112	1.139	1.154
					200.00	1.156	1.134	1.161	1.176
					205.00	1.177	1.156	1.184	1.198
					210.00	1.199	1.178	1.206	1.220
					215.00	1.226	1.200	1.228	1.242
					220.00	1.251	1.223	1.250	1.264
					225.00	1.276	1.245	1.272	1.287
					230.00	1.302	1.267	1.294	1.309
					235.00	1.330	1.289	1.316	1.331
					240.00	1.361	1.311	1.338	1.353
					245.00	1.388	1.333	1.360	1.375
					250.00	1.419	1.355	1.382	1.396
Hexadecanoic Acid	C16H32O2	256.43	0.195	Training set 1, Training set 2	60.00	0.456	0.435	0.452	0.475
					80.00	0.603	0.564	0.585	0.603
					100.00	0.713	0.673	0.697	0.713
					120.00	0.806	0.773	0.799	0.813

					140.00	0.892	0.868	0.894	0.908
					160.00	0.976	0.960	0.987	1.000
					180.00	1.057	1.050	1.078	1.090
					200.00	1.146	1.140	1.167	1.179
					220.00	1.238	1.228	1.256	1.268
					240.00	1.342	1.316	1.344	1.356
Heptadecanoic Acid	C17H34O2	270.45	0.196	Training set 1, Training set 2	90.00	0.660	0.624	0.647	0.661
					95.00	0.687	0.651	0.674	0.688
					100.00	0.713	0.677	0.701	0.715
					105.00	0.737	0.703	0.727	0.740
					110.00	0.761	0.728	0.753	0.766
					115.00	0.786	0.753	0.778	0.791
					120.00	0.809	0.777	0.803	0.815
					125.00	0.829	0.802	0.827	0.839
					130.00	0.853	0.825	0.851	0.863
					135.00	0.875	0.849	0.875	0.887
					140.00	0.897	0.873	0.899	0.910
					145.00	0.917	0.896	0.922	0.933
					150.00	0.938	0.919	0.946	0.956

					155.00	0.958	0.942	0.969	0.979
					160.00	0.978	0.965	0.992	1.002
					165.00	0.998	0.987	1.015	1.025
					170.00	1.019	1.010	1.037	1.048
					175.00	1.041	1.033	1.060	1.070
					180.00	1.062	1.055	1.083	1.093
					185.00	1.082	1.078	1.105	1.115
					190.00	1.104	1.100	1.128	1.138
					195.00	1.124	1.122	1.150	1.160
					200.00	1.147	1.145	1.172	1.182
					205.00	1.171	1.167	1.195	1.204
					210.00	1.192	1.189	1.217	1.227
					215.00	1.217	1.211	1.239	1.249
					220.00	1.242	1.233	1.261	1.271
					225.00	1.267	1.255	1.284	1.293
					230.00	1.296	1.278	1.306	1.315
					235.00	1.322	1.300	1.328	1.337
					240.00	1.351	1.322	1.350	1.359
					245.00	1.384	1.344	1.372	1.381

					250.00	1.406	1.366	1.394	1.403
					255.00	1.436	1.388	1.416	1.425
					260.00	1.468	1.410	1.438	1.447
Octadecanoic Acid	C18H36O2	284.48	0.197	Training set 1, Training set 2	100.00	0.712	0.680	0.705	0.716
					105.00	0.737	0.706	0.731	0.742
					110.00	0.761	0.732	0.757	0.767
					115.00	0.783	0.756	0.782	0.792
					120.00	0.806	0.781	0.807	0.817
					125.00	0.829	0.805	0.831	0.841
					130.00	0.851	0.829	0.855	0.865
					135.00	0.871	0.853	0.879	0.889
					140.00	0.893	0.876	0.903	0.912
					145.00	0.913	0.900	0.927	0.935
					150.00	0.933	0.923	0.950	0.959
					155.00	0.954	0.946	0.973	0.982
					160.00	0.975	0.969	0.996	1.005
					165.00	0.995	0.992	1.019	1.027
					170.00	1.015	1.014	1.042	1.050
					175.00	1.036	1.037	1.065	1.073

					180.00	1.057	1.060	1.087	1.095
					185.00	1.078	1.082	1.110	1.118
					190.00	1.101	1.104	1.132	1.140
					195.00	1.124	1.127	1.155	1.163
					200.00	1.147	1.149	1.177	1.185
					205.00	1.169	1.171	1.199	1.207
					210.00	1.193	1.194	1.222	1.229
					215.00	1.218	1.216	1.244	1.252
					220.00	1.243	1.238	1.266	1.274
					225.00	1.270	1.260	1.288	1.296
					230.00	1.298	1.282	1.311	1.318
					235.00	1.327	1.304	1.333	1.340
					240.00	1.359	1.326	1.355	1.362
					245.00	1.391	1.349	1.377	1.384
					250.00	1.425	1.371	1.399	1.406
					255.00	1.456	1.393	1.421	1.428
					260.00	1.480	1.415	1.443	1.450
					265.00	1.503	1.437	1.465	1.472
					270.00	1.537	1.459	1.487	1.494

Nonadecanoic Acid	C29H38O2	298.51	0.198	Training set 1, Training set 2	90.00	0.658	0.630	0.653	0.664
					95.00	0.685	0.657	0.681	0.691
					100.00	0.711	0.683	0.708	0.717
					105.00	0.736	0.709	0.734	0.743
					110.00	0.759	0.735	0.760	0.769
					115.00	0.783	0.760	0.785	0.794
					120.00	0.806	0.784	0.810	0.818
					125.00	0.829	0.809	0.835	0.843
					130.00	0.849	0.833	0.859	0.867
					135.00	0.872	0.856	0.883	0.890
					140.00	0.892	0.880	0.907	0.914
					145.00	0.913	0.903	0.930	0.937
					150.00	0.933	0.927	0.954	0.961
					155.00	0.956	0.950	0.977	0.984
					160.00	0.975	0.973	1.000	1.007
					165.00	0.994	0.995	1.023	1.029
					170.00	1.015	1.018	1.046	1.052
					175.00	1.037	1.041	1.069	1.075
					180.00	1.057	1.063	1.091	1.097

					185.00	1.078	1.086	1.114	1.120
					190.00	1.099	1.108	1.136	1.142
					195.00	1.121	1.131	1.159	1.165
					200.00	1.144	1.153	1.181	1.187
					205.00	1.166	1.175	1.204	1.209
					210.00	1.188	1.198	1.226	1.232
					215.00	1.214	1.220	1.248	1.254
					220.00	1.238	1.242	1.271	1.276
					225.00	1.263	1.264	1.293	1.298
Eicosanoic Acid	C20H40O2	312.54	0.198	Test set 1, Training set 2	90.00	0.657	0.632	0.656	0.665
					95.00	0.683	0.659	0.683	0.692
					100.00	0.709	0.686	0.710	0.719
					105.00	0.734	0.712	0.737	0.745
					110.00	0.757	0.738	0.763	0.770
					115.00	0.781	0.763	0.788	0.795
					120.00	0.803	0.787	0.813	0.820
					125.00	0.826	0.812	0.838	0.844
					130.00	0.849	0.836	0.862	0.868
					135.00	0.868	0.860	0.886	0.892

					140.00	0.889	0.883	0.910	0.916
					145.00	0.910	0.907	0.933	0.939
					150.00	0.930	0.930	0.957	0.962
					155.00	0.951	0.953	0.980	0.985
					160.00	0.973	0.976	1.003	1.008
					165.00	0.991	0.999	1.026	1.031
					170.00	1.010	1.022	1.049	1.054
					175.00	1.032	1.044	1.072	1.077
					180.00	1.052	1.067	1.095	1.099
					185.00	1.072	1.089	1.117	1.122
					190.00	1.095	1.112	1.140	1.145
					195.00	1.116	1.134	1.162	1.167
					200.00	1.138	1.157	1.185	1.189
					205.00	1.162	1.179	1.207	1.212
					210.00	1.184	1.201	1.230	1.234
					215.00	1.209	1.224	1.252	1.256
					220.00	1.235	1.246	1.274	1.278
					225.00	1.259	1.268	1.297	1.301
					230.00	1.282	1.290	1.319	1.323

					235.00	1.311	1.312	1.341	1.345
					240.00	1.338	1.335	1.363	1.367
					245.00	1.365	1.357	1.385	1.389
					250.00	1.394	1.379	1.407	1.411
					255.00	1.424	1.401	1.430	1.433
					260.00	1.454	1.423	1.452	1.456
					265.00	1.488	1.445	1.474	1.478
					270.00	1.520	1.467	1.496	1.500

Triglycerides									
					50.00	0.355	0.352		0.390
					60.00	0.440	0.427		0.465
					70.00	0.513	0.494		0.532
					80.00	0.575	0.554		0.592
					90.00	0.629	0.610		0.648
					100.00	0.677	0.662		0.700
					110.00	0.722	0.712		0.750
				Test set 1, Training set 2	120.00	0.765	0.761		0.799
b-Tripalmitin	C51H98O6	807.32	0.192		130.00	0.807	0.809	N/A	0.846

					140.00	0.848	0.855		0.893
					150.00	0.870	0.901		0.939
					160.00	0.928	0.946		0.984
					170.00	0.966	0.991		1.029
					180.00	1.006	1.036		1.074
					190.00	1.046	1.080		1.118
					200.00	1.087	1.124		1.162
					210.00	1.130	1.169		1.206
					220.00	1.174	1.213		1.250
					230.00	1.221	1.256		1.294
					240.00	1.271	1.300		1.338
					250.00	1.322	1.344		1.382
					50.00	0.370	0.345		0.379
					55.00	0.420	0.383		0.417
					60.00	0.460	0.419		0.453
					65.00	0.500	0.452		0.487
					70.00	0.530	0.484		0.518
					75.00	0.570	0.514		0.549
					80.00	0.600	0.543		0.578

b-Trielaidin	C57H104O6	885.40	0.189	Test set 1, Training set 2	85.00	0.630	0.571	N/A	0.605
					90.00	0.660	0.598		0.632
					95.00	0.690	0.624		0.659
					100.00	0.720	0.650		0.684
					105.00	0.740	0.675		0.709
					110.00	0.760	0.699		0.734
					120.00	0.810	0.747		0.782
					130.00	0.860	0.794		0.829
					140.00	0.890	0.840		0.875
					150.00	0.930	0.885		0.920
					160.00	0.980	0.930		0.965
					170.00	1.030	0.975		1.009
					180.00	1.070	1.019		1.054
					190.00	1.120	1.063		1.098
					200.00	1.170	1.107		1.142
					210.00	1.210	1.151		1.185
					220.00	1.260	1.195		1.229
					230.00	1.310	1.238		1.273
					240.00	1.370	1.282		1.316

					250.00	1.430	1.325		1.360
b-Tristearin	C57H110O6	891.48	0.194	Test set 1, Training set 2	50.00	0.338	0.356	N/A	0.391
					60.00	0.428	0.433		0.467
					70.00	0.510	0.500		0.534
					80.00	0.575	0.561		0.595
					90.00	0.628	0.617		0.651
					100.00	0.671	0.670		0.704
					110.00	0.697	0.721		0.755
					120.00	0.743	0.770		0.804
					130.00	0.796	0.817		0.852
					140.00	0.817	0.864		0.898
					150.00	0.867	0.910		0.944
					160.00	0.915	0.956		0.990
					170.00	0.955	1.001		1.035
					180.00	0.994	1.046		1.080
					190.00	1.056	1.091		1.125
					200.00	1.109	1.135		1.169
					210.00	1.148	1.179		1.213
					220.00	1.174	1.223		1.258

					230.00	1.210	1.267		1.302
					240.00	1.262	1.311		1.346
					250.00	1.317	1.355		1.390

Naphthene									
Cyclohexyl Formate	C7H12O2	128.17	0.164	Test set 1, Training set 2	50.00	0.384	0.294	0.281	0.373
					60.00	0.441	0.356	0.342	0.436
					70.00	0.492	0.413	0.397	0.492
					80.00	0.539	0.464	0.448	0.544
					90.00	0.584	0.513	0.496	0.592
					100.00	0.628	0.559	0.542	0.638
					110.00	0.672	0.603	0.586	0.682
					120.00	0.717	0.646	0.629	0.726
					130.00	0.764	0.689	0.672	0.768
					135.00	0.801	0.710	0.693	0.789
					140.00	1.105	0.731	0.714	0.810
					145.00	1.449	0.752	0.734	0.831
					150.00	1.458	0.772	0.755	0.852

					160.00	1.465	0.814	0.796	0.893
					170.00	1.471	0.855	0.837	0.934
					180.00	1.479	0.896	0.878	0.975
					190.00	1.490	0.937	0.919	1.016
					200.00	1.505	0.978	0.960	1.057
					201.33	1.507	0.983	0.966	1.063
Cyclohexyl Acatate	C8H14O2	142.20	0.169	Test set 1, Training set 2	50.00	0.356	0.304	0.289	0.375
					60.00	0.423	0.369	0.352	0.440
					70.00	0.481	0.427	0.409	0.498
					80.00	0.537	0.480	0.461	0.551
					90.00	0.589	0.529	0.511	0.601
					100.00	0.633	0.577	0.557	0.648
					110.00	0.679	0.622	0.603	0.694
					120.00	0.722	0.666	0.647	0.738
					130.00	0.764	0.710	0.690	0.781
					140.00	0.805	0.753	0.733	0.824
					150.00	0.847	0.795	0.775	0.867
					160.00	0.887	0.837	0.817	0.909
					170.00	0.927	0.879	0.859	0.951

					180.00	0.971	0.921	0.901	0.992
					190.00	1.014	0.962	0.942	1.034
					200.00	1.057	1.004	0.984	1.076
					210.00	1.100	1.046	1.025	1.117
					220.00	1.143	1.087	1.067	1.159
					221.80	1.150	1.095	1.075	1.166
trans-Hexahydroindan	C9H16	124.22	0.201	Test set 1, Training set 2	50.00	0.354	0.372	0.345	0.372
					60.00	0.409	0.451	0.421	0.451
					70.00	0.458	0.521	0.488	0.521
					80.00	0.500	0.584	0.549	0.584
					90.00	0.543	0.642	0.606	0.642
					100.00	0.583	0.697	0.659	0.697
					110.00	0.622	0.749	0.710	0.749
					120.00	0.662	0.799	0.760	0.799
					130.00	0.701	0.848	0.809	0.848
					140.00	0.741	0.896	0.856	0.896
					150.00	0.779	0.943	0.903	0.943
					160.00	0.820	0.989	0.949	0.989
					170.00	0.859	1.035	0.995	1.035

					180.00	0.901	1.081	1.040	1.081
					190.00	0.947	1.126	1.085	1.126
					200.00	0.992	1.171	1.130	1.171
					210.00	1.037	1.216	1.175	1.216
					213.86	1.055	1.233	1.192	1.233
Butylcyclopentane	C9H18	126.24	0.214	Training set 1, Training set 2	50.00	0.435	0.399	0.374	0.399
					60.00	0.521	0.484	0.453	0.484
					70.00	0.596	0.559	0.524	0.559
					80.00	0.664	0.626	0.587	0.626
					90.00	0.725	0.687	0.646	0.687
					100.00	0.779	0.744	0.701	0.744
					110.00	0.830	0.799	0.754	0.799
					120.00	0.881	0.851	0.806	0.851
					130.00	0.929	0.902	0.855	0.902
					140.00	0.978	0.951	0.904	0.951
					150.00	1.032	1.000	0.952	1.000
					160.00	1.091	1.048	0.999	1.048
					165.18	1.122	1.072	1.024	1.072
trans-	C10H18	138.25	0.203	Test set 1, Training	50.00	0.289	0.375	0.348	0.375

Decahydronaphtalene				set 2	60.00	0.341	0.455	0.423	0.455
					70.00	0.389	0.525	0.491	0.525
					80.00	0.434	0.588	0.552	0.588
					90.00	0.480	0.647	0.609	0.647
					100.00	0.522	0.702	0.663	0.702
					110.00	0.566	0.754	0.715	0.754
					120.00	0.610	0.804	0.765	0.804
					130.00	0.654	0.853	0.813	0.853
					140.00	0.698	0.901	0.861	0.901
					150.00	0.741	0.949	0.908	0.949
					160.00	0.785	0.995	0.954	0.995
					170.00	0.829	1.041	1.000	1.041
					180.00	0.874	1.087	1.045	1.087
					190.00	0.920	1.132	1.091	1.132
					200.00	0.966	1.178	1.136	1.178
					210.00	1.015	1.223	1.181	1.223
					220.00	1.065	1.267	1.225	1.267
					230.00	1.117	1.312	1.270	1.312
					240.00	1.172	1.357	1.314	1.357

					242.78	1.188	1.369	1.327	1.369
Cycloheyl butyrate	C10H18O2	170.25	0.176	Training set 1, Training set 2	50.00	0.361	0.319	0.307	0.379
					60.00	0.425	0.387	0.372	0.447
					70.00	0.483	0.448	0.431	0.508
					80.00	0.536	0.503	0.485	0.563
					90.00	0.586	0.555	0.535	0.615
					100.00	0.631	0.604	0.583	0.664
					110.00	0.676	0.651	0.629	0.711
					120.00	0.721	0.697	0.675	0.756
					130.00	0.763	0.741	0.719	0.801
					140.00	0.807	0.785	0.763	0.845
					150.00	0.850	0.829	0.806	0.889
					160.00	0.890	0.872	0.849	0.932
					170.00	0.929	0.915	0.892	0.975
					180.00	0.969	0.958	0.934	1.018
					190.00	1.009	1.001	0.977	1.060
					200.00	1.049	1.043	1.019	1.103
					210.00	1.088	1.086	1.062	1.145
					219.60	1.126	1.126	1.102	1.186

Butylcyclohexane	C10H20	140.27	0.214	Training set 1, Training set 2	50.00	0.384	0.399	0.374	0.399
					60.00	0.457	0.484	0.453	0.484
					70.00	0.524	0.559	0.524	0.559
					80.00	0.585	0.626	0.587	0.626
					90.00	0.644	0.687	0.646	0.687
					100.00	0.694	0.744	0.701	0.744
					110.00	0.746	0.799	0.754	0.799
					120.00	0.795	0.851	0.806	0.851
					130.00	0.842	0.902	0.855	0.902
					140.00	0.889	0.951	0.904	0.951
					150.00	0.935	1.000	0.952	1.000
					160.00	0.982	1.048	0.999	1.048
					170.00	1.028	1.095	1.046	1.095
					180.00	1.076	1.142	1.093	1.142
					190.00	1.122	1.188	1.139	1.188
					198.42	1.162	1.227	1.177	1.227
Cyclohexyl valerate	C11H20O2	184.28	0.179	Training set 1, Training set 2	50.00	0.360	0.325	0.312	0.380
					60.00	0.426	0.394	0.378	0.450
					70.00	0.485	0.456	0.438	0.511

					80.00	0.540	0.512	0.492	0.568
					90.00	0.592	0.565	0.544	0.620
					100.00	0.640	0.614	0.592	0.670
					110.00	0.685	0.662	0.639	0.717
					120.00	0.728	0.708	0.685	0.763
					130.00	0.770	0.754	0.730	0.809
					140.00	0.810	0.798	0.774	0.853
					150.00	0.852	0.842	0.817	0.897
					160.00	0.896	0.886	0.861	0.941
					170.00	0.942	0.929	0.904	0.984
					180.00	0.989	0.972	0.947	1.027
					190.00	1.037	1.015	0.990	1.070
					200.00	1.084	1.058	1.032	1.113
					210.00	1.131	1.101	1.075	1.156
					220.00	1.177	1.144	1.118	1.199
					222.40	1.188	1.154	1.128	1.209
trans-e-Cyclohexylcyclohexanol	C12H22O	182.30	0.192	Training set 1, Training set 2	50.00	0.294	0.352	0.335	0.380
					60.00	0.344	0.427	0.406	0.455
					70.00	0.395	0.494	0.470	0.522

					80.00	0.439	0.554	0.528	0.582
					90.00	0.484	0.610	0.582	0.638
					100.00	0.528	0.662	0.633	0.690
					110.00	0.571	0.712	0.682	0.740
					120.00	0.612	0.761	0.730	0.789
					130.00	0.653	0.808	0.777	0.836
					140.00	0.694	0.855	0.823	0.883
					150.00	0.737	0.901	0.868	0.929
					160.00	0.779	0.946	0.913	0.974
					170.00	0.821	0.991	0.958	1.019
					180.00	0.859	1.036	1.002	1.064
					190.00	0.893	1.080	1.047	1.108
					200.00	0.931	1.124	1.091	1.152
					210.00	0.972	1.169	1.135	1.196
					220.00	1.015	1.213	1.178	1.240
					230.00	1.059	1.256	1.222	1.284
					240.00	1.104	1.300	1.266	1.328
					250.00	1.149	1.344	1.310	1.372
					260.00	1.194	1.388	1.353	1.416

					270.00	1.238	1.432	1.397	1.460
					280.00	1.283	1.475	1.441	1.503
					290.00	1.328	1.519	1.485	1.547
					298.15	1.364	1.555	1.520	1.583
					300.00	1.372	1.563	1.528	1.591
					310.00	1.417	1.607	1.572	1.635
					320.00	1.461	1.651	1.616	1.678
Heptylcyclohexane	C13H26	182.35	0.214	Training set 1, Training set 2	80.00	0.599	0.626	0.587	0.626
					90.00	0.651	0.687	0.646	0.687
					100.00	0.703	0.744	0.701	0.744
					110.00	0.754	0.799	0.754	0.799
					120.00	0.804	0.851	0.806	0.851
					130.00	0.856	0.902	0.855	0.902
					140.00	0.912	0.951	0.904	0.951
					150.00	0.968	1.000	0.952	1.000
					160.00	1.008	1.048	0.999	1.048
					170.00	1.046	1.095	1.046	1.095
					180.00	1.100	1.142	1.093	1.142
					190.00	1.167	1.188	1.139	1.188

Pentadecanolactone	C15H28O2	240.39	0.187	Training set 1, Training set 2	50.00	0.323	0.342	0.326	0.384
					100.00	0.602	0.644	0.618	0.687
					150.00	0.815	0.879	0.850	0.921
					200.00	1.032	1.100	1.069	1.142
					250.00	1.266	1.318	1.287	1.360
					282.98	1.421	1.461	1.430	1.503
Decylcyclopentane	C15H30	210.40	0.214	Training set 1, Training set 2	50.00	0.399	0.399	0.374	0.399
					60.00	0.480	0.484	0.453	0.484
					70.00	0.553	0.559	0.524	0.559
					80.00	0.620	0.626	0.587	0.626
					90.00	0.681	0.687	0.646	0.687
					100.00	0.733	0.744	0.701	0.744
					110.00	0.783	0.799	0.754	0.799
					120.00	0.831	0.851	0.806	0.851
					130.00	0.876	0.902	0.855	0.902
					140.00	0.920	0.951	0.904	0.951
					150.00	0.964	1.000	0.952	1.000
					160.00	1.007	1.048	0.999	1.048
					170.00	1.051	1.095	1.046	1.095

					180.00	1.098	1.142	1.093	1.142
					190.00	1.147	1.188	1.139	1.188
					200.00	1.198	1.234	1.184	1.234
					210.00	1.258	1.280	1.230	1.280
					220.00	1.325	1.325	1.275	1.325
					230.00	1.400	1.370	1.320	1.370
trans,trans,-4-Propylbicyclohexyl	C16H27N	233.39	0.189	Test set 1, Training set 2	50.00	0.306	0.345	0.323	0.364
					60.00	0.369	0.418	0.394	0.438
					70.00	0.427	0.484	0.457	0.503
					80.00	0.481	0.543	0.515	0.562
					90.00	0.531	0.598	0.568	0.617
					100.00	0.579	0.649	0.620	0.668
					110.00	0.625	0.699	0.669	0.718
					120.00	0.670	0.747	0.716	0.766
					130.00	0.713	0.794	0.763	0.813
					140.00	0.756	0.840	0.808	0.859
					150.00	0.798	0.885	0.854	0.904
					160.00	0.840	0.930	0.898	0.949
					170.00	0.882	0.975	0.943	0.994

					180.00	0.922	1.019	0.987	1.038
					190.00	0.964	1.063	1.031	1.082
					200.00	1.006	1.107	1.075	1.126
					210.00	1.049	1.151	1.118	1.170
					220.00	1.093	1.194	1.162	1.213
					230.00	1.140	1.238	1.205	1.257
					240.00	1.186	1.281	1.249	1.300
					250.00	1.234	1.325	1.293	1.344
					260.00	1.285	1.369	1.336	1.388
					270.00	1.339	1.412	1.380	1.431
					280.00	1.393	1.456	1.423	1.475
					290.00	1.450	1.499	1.467	1.518
					300.00	1.510	1.543	1.510	1.562
					310.00	1.570	1.587	1.554	1.606
					320.00	1.651	1.630	1.598	1.649
Decyclohexane	C16H32	224.43	0.214	Training set 1, Training set 2	50.00	0.366	0.399	0.374	0.399
					60.00	0.441	0.484	0.453	0.484
					70.00	0.509	0.559	0.524	0.559
					80.00	0.572	0.626	0.587	0.626

					90.00	0.630	0.687	0.646	0.687
					100.00	0.680	0.744	0.701	0.744
					110.00	0.728	0.799	0.754	0.799
					120.00	0.774	0.851	0.806	0.851
					130.00	0.818	0.902	0.855	0.902
					140.00	0.861	0.951	0.904	0.951
					150.00	0.902	1.000	0.952	1.000
					160.00	0.944	1.048	0.999	1.048
					170.00	0.985	1.095	1.046	1.095
					180.00	1.027	1.142	1.093	1.142
					190.00	1.069	1.188	1.139	1.188
					200.00	1.113	1.234	1.184	1.234
					210.00	1.157	1.280	1.230	1.280
					220.00	1.204	1.325	1.275	1.325
					230.00	1.253	1.370	1.320	1.370
					240.00	1.303	1.415	1.365	1.415
					250.00	1.367	1.460	1.410	1.460
					260.00	1.413	1.505	1.455	1.505
					270.00	1.473	1.550	1.499	1.550

					271.43	1.483	1.556	1.505	1.556
Dodecycloheca ne	C18H36	252.48	0.214	Test set 1, Training set 2	80.00	0.581	0.626	0.583	0.626
					90.00	0.633	0.687	0.642	0.687
					100.00	0.682	0.744	0.698	0.744
					110.00	0.729	0.799	0.752	0.799
					120.00	0.776	0.851	0.803	0.851
					130.00	0.823	0.902	0.853	0.902
					140.00	0.867	0.951	0.902	0.951
					150.00	0.909	1.000	0.951	1.000
					160.00	0.952	1.048	0.998	1.048
					170.00	0.995	1.095	1.045	1.095
					180.00	1.040	1.142	1.092	1.142
					190.00	1.087	1.188	1.138	1.188
					200.00	1.138	1.234	1.184	1.234
					210.00	1.187	1.280	1.229	1.280
					220.00	1.236	1.325	1.274	1.325
					230.00	1.301	1.370	1.320	1.370
Cholesterol	C27H46O	386.66	0.191	Test set 1, Training set 2	50.00	0.320	0.426		0.364
					60.00	0.320	0.426	0.400	0.439

					70.00	0.373	0.492	0.464	0.505
					80.00	0.425	0.552	0.522	0.565
					90.00	0.477	0.608	0.577	0.621
					100.00	0.528	0.660	0.628	0.673
					110.00	0.579	0.710	0.678	0.723
					120.00	0.628	0.759	0.726	0.772
					130.00	0.673	0.806	0.773	0.819
					140.00	0.721	0.852	0.819	0.865
					150.00	0.765	0.898	0.865	0.911
					160.00	0.809	0.943	0.910	0.957
					170.00	0.853	0.988	0.955	1.001
					180.00	0.903	1.033	0.999	1.046
					190.00	0.949	1.077	1.043	1.090
					200.00	0.997	1.121	1.087	1.134
					210.00	1.045	1.165	1.131	1.179
					220.00	1.093	1.209	1.175	1.222
					230.00	1.143	1.253	1.219	1.266
					240.00	1.194	1.297	1.263	1.310
					250.00	1.245	1.341	1.306	1.354

					260.00	1.297	1.385	1.350	1.398
					270.00	1.352	1.428	1.394	1.441
					280.00	1.413	1.472	1.438	1.485
					80.00	0.590	0.626	0.583	0.626
					90.00	0.653	0.687	0.642	0.687
					100.00	0.703	0.744	0.698	0.744
					110.00	0.748	0.799	0.752	0.799
					120.00	0.796	0.851	0.803	0.851
11-Cyclohexylhen eicosane	C27H54	378.72	0.214	Test set 1, Training set 2	130.00	0.843	0.902	0.853	0.902
					140.00	0.889	0.951	0.902	0.951
					150.00	0.935	1.000	0.951	1.000
					160.00	0.981	1.048	0.998	1.048
					170.00	1.019	1.095	1.045	1.095
					180.00	1.062	1.142	1.092	1.142
					190.00	1.112	1.188	1.138	1.188
					200.00	1.162	1.234	1.184	1.234
					210.00	1.213	1.280	1.229	1.280
					220.00	1.263	1.325	1.274	1.325
					230.00	1.324	1.370	1.320	1.370

					240.00	1.397	1.415	1.365	1.415
					250.00	1.498	1.460	1.409	1.460

Compounds with heteroatom (SNO)									
Isoquinoline	C9H7N	129.16	0.132	Test set 1, Training set 2	50.00	0.287	0.230	N/A	0.297
					60.00	0.329	0.279		0.353
					70.00	0.369	0.323		0.403
					80.00	0.403	0.365		0.450
					90.00	0.435	0.405		0.494
					100.00	0.465	0.443		0.536
					110.00	0.496	0.480		0.577
					120.00	0.530	0.516		0.618
					130.00	0.562	0.552		0.657
					140.00	0.595	0.588		0.696
					150.00	0.629	0.624		0.735
					160.00	0.664	0.660		0.774
					170.00	0.700	0.695		0.812
					180.00	0.737	0.731		0.851

Quinoline	C9H7N	129.16	0.132	Test set 1, Training set 2	50.00	0.296	0.230		0.890
					60.00	0.340	0.279		0.928
					70.00	0.377	0.323		0.967
					80.00	0.411	0.365		1.006
					90.00	0.443	0.405		1.045
					100.00	0.474	0.443		1.084
					110.00	0.506	0.480		1.123
					120.00	0.538	0.516		1.163
					130.00	0.571	0.552		1.202
					140.00	0.604	0.588		1.242
					150.00	0.638	0.624		1.282
					160.00	0.674	0.660		1.322
					170.00	0.710	0.695		0.730
					180.00	0.746	0.731		0.765
					190.00	0.783	0.767		0.801
					200.00	0.820	0.803		0.837
					205.00	0.840	0.821		0.855
					210.00	0.860	0.839		0.873
					215.00	0.880	0.857		0.891

					220.00	0.901	0.875		0.909
Carbazole	C12H9N	167.21	0.132	Test set 1, Training set 2	180.00	0.724	0.731		0.757
					185.00	0.739	0.749		0.775
					190.00	0.754	0.766		0.793
					195.00	0.770	0.784		0.811
					200.00	0.785	0.802		0.829
					205.00	0.801	0.820		0.847
					210.00	0.818	0.838		0.865
					215.00	0.834	0.856		0.883
					220.00	0.851	0.874		0.901
					225.00	0.868	0.893		0.919
					230.00	0.885	0.911		0.937
					235.00	0.902	0.929		0.956
					240.00	0.920	0.947		0.974
					245.00	0.938	0.966		0.992
					250.00	0.956	0.984		1.011
					255.00	0.974	1.002		1.029
					260.00	0.992	1.021		1.047
					265.00	1.011	1.039		1.066

					270.00	1.030	1.058		1.085
					275.00	1.049	1.077		1.103
					280.00	1.069	1.095		1.122
					285.00	1.088	1.114		1.141
					290.00	1.108	1.133		1.159
					295.00	1.128	1.152		1.178
					300.00	1.148	1.170		1.197
					305.00	1.169	1.189		1.216
					310.00	1.189	1.208		1.235
					315.00	1.210	1.227		1.254
					320.00	1.232	1.246		1.273
					325.00	1.253	1.266		1.292
					330.00	1.275	1.285		1.311
					335.00	1.296	1.304		1.331
					340.00	1.318	1.323		1.350
					345.00	1.341	1.343		1.369
					350.00	1.363	1.362		1.389
					355.00	1.386	1.382		1.408
					360.00	1.409	1.401		1.428

					365.00	1.432	1.421		1.447
					370.00	1.455	1.440		1.467
					375.00	1.479	1.460		1.487
					380.00	1.503	1.480		1.506
					385.00	1.527	1.500		1.526
					390.00	1.551	1.519		1.546
					395.00	1.576	1.539		1.566
					400.00	1.601	1.559		1.586
Phenoxathiin	C12H8OS	200.26	0.110	Test set 1, Training set 2	50.00	0.235	0.188		0.264
					60.00	0.272	0.228		0.304
					70.00	0.305	0.265		0.341
					80.00	0.337	0.300		0.376
					90.00	0.368	0.334		0.410
					100.00	0.399	0.366		0.442
					120.00	0.460	0.429		0.505
					140.00	0.523	0.492		0.568
					160.00	0.588	0.554		0.630
					180.00	0.654	0.616		0.692
					200.00	0.722	0.679		0.756

					220.00	0.791	0.743		0.819
					240.00	0.862	0.808		0.884
					260.00	0.933	0.873		0.949
					280.00	1.003	0.940		1.016
					298.15	1.067	1.001		1.077
					300.00	1.074	1.007		1.083
Dibenzothiophene	C12H8S	184.26	0.114	Training set 1, Training set 2	60.00	0.270	0.238		0.293
					80.00	0.337	0.312		0.368
					100.00	0.399	0.380		0.436
					120.00	0.460	0.446		0.501
					140.00	0.523	0.510		0.565
					160.00	0.588	0.574		0.629
					180.00	0.654	0.638		0.693
					200.00	0.724	0.703		0.758
					250.00	0.902	0.868		0.923
					298.15	1.076	1.032		1.088
					300.00	1.083	1.039		1.094
					350.00	1.264	1.215		1.271
					371.82	1.346	1.294		1.350

Thianthrene	C12H8S2	216.32	0.102	Training set 1, Training set 2	40.00	0.178	0.133		0.227
					50.00	0.219	0.173		0.267
					60.00	0.256	0.210		0.304
					70.00	0.290	0.244		0.338
					80.00	0.322	0.276		0.370
					90.00	0.354	0.307		0.401
					100.00	0.386	0.338		0.432
					120.00	0.448	0.397		0.491
					140.00	0.510	0.455		0.549
					160.00	0.573	0.514		0.608
					180.00	0.636	0.573		0.667
					200.00	0.700	0.632		0.726
					220.00	0.765	0.693		0.787
					240.00	0.830	0.754		0.848
					260.00	0.895	0.816		0.910
					280.00	0.960	0.879		0.973
					300.00	1.024	0.943		1.037
					320.00	1.087	1.007		1.101
					340.00	1.149	1.073		1.167

					360.00	1.210	1.140		1.234
					380.00	1.270	1.208		1.302
					400.00	1.328	1.277		1.371
					420.00	1.384	1.347		1.441
					429.58	1.410	1.381		1.475
trans-Azobenzene	C12H10N2	182.22	0.132	Training set 1, Training set 2	90.00	0.460	0.405		0.454
					100.00	0.491	0.443		0.492
					110.00	0.526	0.480		0.529
					120.00	0.561	0.517		0.565
					130.00	0.595	0.553		0.602
					140.00	0.629	0.589		0.637
					150.00	0.664	0.624		0.673
					160.00	0.699	0.660		0.709
					170.00	0.734	0.696		0.744
					180.00	0.770	0.731		0.780
					190.00	0.808	0.767		0.816
					200.00	0.846	0.803		0.852
					210.00	0.884	0.839		0.888
					220.00	0.924	0.875		0.924

					230.00	0.962	0.912		0.960
Diphenylsulfide	C12H10S	186.27	0.123	Training set 1, Training set 2	50.00	0.292	0.214		0.268
					60.00	0.335	0.260		0.314
					70.00	0.374	0.301		0.356
					80.00	0.409	0.341		0.395
					90.00	0.443	0.378		0.432
					100.00	0.476	0.414		0.468
					120.00	0.540	0.484		0.538
					140.00	0.605	0.552		0.607
					160.00	0.672	0.620		0.675
					180.00	0.742	0.688		0.743
					200.00	0.816	0.757		0.811
					220.00	0.893	0.826		0.881
					240.00	0.973	0.896		0.951
					250.00	1.014	0.931		0.986
					257.80	1.045	0.959		1.014
2-Aminobiphenyl	C12H11N	169.22	0.142	Test set 1, Training set 2	50.00	0.299	0.340		0.276
					60.00	0.346	0.359		0.329
					70.00	0.388	0.377		0.378

					80.00	0.426	0.395		0.422
					90.00	0.463	0.413		0.465
					100.00	0.499	0.431		0.505
					110.00	0.535	0.250		0.545
					120.00	0.570	0.303		0.584
					130.00	0.606	0.351		0.622
					140.00	0.643	0.396		0.660
					150.00	0.680	0.438		0.697
					160.00	0.717	0.479		0.735
					170.00	0.755	0.519		0.773
					180.00	0.794	0.557		0.810
					190.00	0.834	0.596		0.848
					200.00	0.874	0.633		0.885
					210.00	0.915	0.671		0.923
					220.00	0.956	0.709		0.961
					230.00	0.999	0.746		0.999
					240.00	1.043	0.784		1.037
					245.00	1.066	0.821		1.056
					250.00	1.092	0.859		1.075

					252.00	1.102	0.897		1.083
					254.00	1.113	0.935		1.091
					256.00	1.123	0.973		1.099
					258.00	1.137	1.011		1.106
Carboxin	C12H13NO2S		0.123	Training set 1, Training set 2	80.00	0.343	1.030		0.424
					85.00	0.361	1.049		0.442
					90.00	0.378	1.057		0.461
					95.00	0.394	1.065		0.479
					100.00	0.410	1.072		0.497
					105.00	0.425	1.080		0.515
					110.00	0.439	0.448		0.532
					115.00	0.453	0.466		0.549
					120.00	0.467	0.483		0.567
					125.00	0.481	0.500		0.584
					130.00	0.495	0.517		0.601
					135.00	0.509	0.534		0.618
					140.00	0.524	0.551		0.635
					145.00	0.538	0.568		0.652
					150.00	0.553	0.585		0.669

					155.00	0.568	0.602		0.686
					160.00	0.584	0.619		0.703
					165.00	0.600	0.636		0.720
					170.00	0.616	0.653		0.737
					175.00	0.633	0.670		0.754
					180.00	0.649	0.687		0.771
					185.00	0.666	0.704		0.788
					190.00	0.684	0.721		0.805
					195.00	0.701	0.738		0.822
					200.00	0.719	0.756		0.839
					205.00	0.737	0.773		0.857
					210.00	0.755	0.790		0.874
					215.00	0.773	0.807		0.891
					220.00	0.791	0.825		0.909
					225.00	0.809	0.842		0.926
					230.00	0.827	0.860		0.943
					235.00	0.845	0.877		0.961
					240.00	0.862	0.895		0.978
					245.00	0.880	0.912		0.996

					250.00	0.897	0.930		1.014
					255.00	0.915	0.948		1.031
					260.00	0.932	0.965		1.049
					265.00	0.949	0.983		1.067
					270.00	0.965	1.001		1.085
					275.00	0.982	1.019		1.103
					280.00	0.999	1.037		1.121
					285.00	1.016	1.055		1.139
					290.00	1.033	1.073		1.157
					295.00	1.050	1.091		1.175
					298.15	1.061	1.102		1.186
					300.00	1.068	1.109		1.193
					305.00	1.086	1.127		1.211
					310.00	1.105	1.146		1.229
					315.00	1.125	1.164		1.248
					320.00	1.146	1.182		1.266
					325.00	1.168	1.201		1.285
					330.00	1.191	1.219		1.303
					335.00	1.217	1.238		1.322

					340.00	1.244	1.257		1.340
					345.00	1.274	1.275		1.359
					350.00	1.307	1.294		1.378
					355.00	1.343	1.313		1.397
					360.00	1.382	1.332		1.416
Acridine	C13H9N	179.22	0.128	Training set 1, Training set 2	50.00	0.241	0.223		0.248
					60.00	0.280	0.271		0.296
					70.00	0.315	0.314		0.339
					80.00	0.347	0.355		0.380
					90.00	0.379	0.394		0.419
					100.00	0.409	0.431		0.456
					110.00	0.441	0.467		0.492
					120.00	0.472	0.503		0.528
					130.00	0.505	0.539		0.563
					140.00	0.538	0.574		0.598
					150.00	0.571	0.609		0.634
					160.00	0.606	0.644		0.669
					170.00	0.642	0.679		0.704
					180.00	0.679	0.714		0.739

					190.00	0.716	0.749		0.774
					200.00	0.753	0.784		0.809
					210.00	0.792	0.820		0.844
					220.00	0.831	0.855		0.880
					230.00	0.870	0.891		0.916
					240.00	0.909	0.927		0.952
					250.00	0.950	0.963		0.988
					260.00	0.990	0.999		1.024
					270.00	1.030	1.036		1.061
					280.00	1.071	1.073		1.097
					290.00	1.112	1.110		1.134
					298.15	1.144	1.140		1.165
					300.00	1.152	1.147		1.172
					310.00	1.192	1.184		1.209
					320.00	1.233	1.222		1.247
					330.00	1.275	1.260		1.284
					340.00	1.316	1.298		1.323
					350.00	1.357	1.336		1.361
					360.00	1.399	1.374		1.399

					370.00	1.443	1.413		1.438
					380.00	1.487	1.452		1.477
					383.24	1.501	1.465		1.490
Phenanthridine	C13H9N	179.22	0.128	Training set 1, Training set 2	50.00	0.243	0.223		0.248
					60.00	0.283	0.271		0.296
					70.00	0.317	0.314		0.339
					80.00	0.350	0.355		0.380
					90.00	0.380	0.394		0.419
					100.00	0.410	0.431		0.456
					110.00	0.441	0.467		0.492
					120.00	0.472	0.503		0.528
					130.00	0.503	0.539		0.563
					140.00	0.535	0.574		0.598
					150.00	0.568	0.609		0.634
					160.00	0.602	0.644		0.669
					170.00	0.637	0.679		0.704
					180.00	0.672	0.714		0.739
					190.00	0.708	0.749		0.774
					200.00	0.744	0.784		0.809

					210.00	0.782	0.820		0.844
					220.00	0.820	0.855		0.880
					230.00	0.858	0.891		0.916
					240.00	0.897	0.927		0.952
					250.00	0.936	0.963		0.988
					260.00	0.975	0.999		1.024
					270.00	1.015	1.036		1.061
					280.00	1.054	1.073		1.097
					290.00	1.094	1.110		1.134
					298.15	1.126	1.140		1.165
					300.00	1.134	1.147		1.172
					310.00	1.172	1.184		1.209
					320.00	1.212	1.222		1.247
					330.00	1.252	1.260		1.284
					340.00	1.291	1.298		1.323
					350.00	1.330	1.336		1.361
					354.00	1.346	1.351		1.376
7,8 Benzoquinoline	C13H9N	197.22	0.128	Training set 1, Training set 2	50.00	0.250	0.223		0.248
					60.00	0.288	0.271		0.296

					70.00	0.322	0.314		0.339
					80.00	0.354	0.355		0.380
					90.00	0.385	0.394		0.419
					100.00	0.415	0.431		0.456
					110.00	0.445	0.467		0.492
					120.00	0.476	0.503		0.528
					130.00	0.508	0.539		0.563
					140.00	0.541	0.574		0.598
					150.00	0.573	0.609		0.634
					160.00	0.608	0.644		0.669
					170.00	0.643	0.679		0.704
					180.00	0.679	0.714		0.739
					190.00	0.715	0.749		0.774
					200.00	0.753	0.784		0.809
					210.00	0.791	0.820		0.844
					220.00	0.829	0.855		0.880
					230.00	0.869	0.891		0.916
					240.00	0.908	0.927		0.952
					250.00	0.949	0.963		0.988

					260.00	0.990	0.999		1.024
					270.00	1.031	1.036		1.061
					280.00	1.073	1.073		1.097
					290.00	1.115	1.110		1.134
					298.15	1.151	1.140		1.165
					300.00	1.160	1.147		1.172
					310.00	1.209	1.184		1.209
					320.00	1.260	1.222		1.247
					324.10	1.280	1.237		1.262
Diphenylcarbodiimide	C13H10N2	194.24	0.124	Training set 1, Training set 2	50.00	0.306	0.215		0.261
					100.00	0.499	0.416		0.462
					150.00	0.662	0.590		0.635
					200.00	0.849	0.761		0.807
					250.00	1.045	0.936		0.982
					287.41	1.191	1.070		1.116
N-Methylcarcazole	C13H11N	181.23	0.138	Training set 1, Training set 2	50.00	0.280	0.242		0.266
					60.00	0.324	0.294		0.318
					70.00	0.364	0.341		0.365
					80.00	0.399	0.384		0.409

					90.00	0.433	0.425		0.450
					100.00	0.467	0.465		0.490
					110.00	0.500	0.504		0.528
					120.00	0.532	0.542		0.566
					130.00	0.564	0.579		0.604
					140.00	0.597	0.616		0.641
					150.00	0.630	0.653		0.678
					160.00	0.664	0.690		0.715
					170.00	0.698	0.727		0.751
					180.00	0.734	0.764		0.788
					190.00	0.771	0.801		0.825
					200.00	0.808	0.838		0.862
					210.00	0.846	0.875		0.899
					220.00	0.884	0.912		0.937
					230.00	0.923	0.949		0.974
					240.00	0.962	0.987		1.011
					250.00	1.003	1.025		1.049
					260.00	1.043	1.063		1.087
					270.00	1.084	1.101		1.125

					273.15	1.097	1.113		1.137
					280.00	1.126	1.139		1.163
					290.00	1.168	1.177		1.202
					298.15	1.202	1.209		1.233
					300.00	1.210	1.216		1.241
					310.00	1.252	1.255		1.280
					320.00	1.294	1.294		1.319
					330.00	1.338	1.333		1.358
					340.00	1.382	1.373		1.397
					350.00	1.426	1.413		1.437
					360.00	1.468	1.452		1.477
					362.49	1.480	1.462		1.487
1,2,3,4-tetrahydro-N-Methylcarbazole	C13H15N	185.26	0.157	Test set 1, Training set 2	50.00	0.282	0.385		0.303
					55.00	0.311	0.417		0.333
					60.00	0.339	0.454		0.362
					65.00	0.367	0.522		0.390
					70.00	0.392	0.563		0.416
					75.00	0.416	0.608		0.441
					80.00	0.439	0.279		0.465

					85.00	0.461	0.309		0.489
					90.00	0.482	0.338		0.512
					95.00	0.502	0.366		0.534
					100.00	0.521	0.392		0.556
					102.00	0.529	0.417		0.565
					103.80	0.536	0.441		0.572
9-Fluorenemethanol	C14H12O	196.25	0.138	Test set 1, Training set 2	78.50	0.380	0.465		0.403
					79.90	0.385	0.488		0.409
					82.26	0.393	0.510		0.418
					84.64	0.402	0.532		0.428
					85.94	0.406	0.541		0.434
					87.24	0.411	0.548		0.439
					88.54	0.416	0.377		0.444
					89.84	0.421	0.383		0.450
					91.05	0.425	0.393		0.454
					92.27	0.430	0.402		0.459
					93.81	0.435	0.408		0.465
					95.68	0.442	0.413		0.473
					97.47	0.450	0.418		0.480

					99.25	0.457	0.424		0.487
					101.04	0.463	0.429		0.494
					102.74	0.469	0.433		0.500
					104.45	0.475	0.440		0.507
					106.15	0.481	0.447		0.514
					107.78	0.487	0.454		0.520
					110.05	0.496	0.461		0.529
					112.81	0.506	0.468		0.539
					115.57	0.515	0.475		0.549
					118.25	0.525	0.481		0.560
					120.84	0.535	0.488		0.569
					123.44	0.546	0.494		0.579
					126.04	0.557	0.503		0.589
					128.55	0.566	0.513		0.598
					131.07	0.576	0.524		0.608
					133.51	0.583	0.534		0.617
					135.94	0.594	0.543		0.626
					138.38	0.602	0.553		0.635
					140.73	0.613	0.563		0.643

					143.08	0.621	0.572		0.652
					145.44	0.629	0.582		0.661
					147.79	0.640	0.591		0.669
					150.06	0.649	0.600		0.678
					152.34	0.659	0.609		0.686
					154.61	0.667	0.617		0.694
					156.80	0.675	0.626		0.702
					158.99	0.684	0.635		0.711
					161.18	0.693	0.643		0.719
					163.38	0.701	0.652		0.727
					165.57	0.709	0.660		0.735
					167.68	0.719	0.669		0.742
					169.87	0.727	0.677		0.751
					171.98	0.735	0.685		0.758
					174.09	0.744	0.693		0.766
					176.12	0.753	0.701		0.773
					178.23	0.762	0.709		0.781
					180.26	0.771	0.717		0.789
					182.29	0.781	0.725		0.796

					184.32	#VALUE!	0.732		0.804
					186.35	0.000	0.740		0.811
					188.38	0.000	0.748		0.819
					190.32	0.000	0.755		0.826
					192.27	0.000	0.763		0.833
					194.22	0.000	0.770		0.840
					196.17	0.000	0.778		0.847
					198.12	0.000	0.785		0.855
					200.06	0.000	0.793		0.862
					201.93	0.000	0.800		0.869
					203.88	0.000	0.807		0.876
					205.75	0.000	0.814		0.883
					207.69	0.000	0.821		0.890
					209.56	0.000	0.829		0.897
					211.43	0.000	0.836		0.904
					213.21	0.000	0.843		0.911
					215.08	0.000	0.850		0.917
					216.95	0.000	0.857		0.924
					218.73	0.000	0.864		0.931

					220.52	0.000	0.871		0.938
					222.39	0.000	0.878		0.945
					224.17	0.000	0.885		0.951
					225.96	0.000	0.892		0.958
					227.66	0.000	0.899		0.964
					229.45	0.000	0.905		0.971
					231.15	0.000	0.912		0.977
					232.86	0.000	0.919		0.984
					234.64	0.000	0.925		0.991
					236.35	0.000	0.932		0.997
					238.05	0.000	0.938		1.003
					239.76	0.000	0.945		1.010
					241.46	0.000	0.952		1.016
					243.08	0.000	0.958		1.022
					244.71	0.000	0.965		1.028
					246.41	0.000	0.971		1.035
					248.12	0.000	0.977		1.041
					249.74	0.000	0.984		1.047
					251.36	0.000	0.990		1.053

					253.07	0.000	0.996		1.060
					254.69	0.000	1.002		1.066
					256.31	0.000	1.009		1.072
					257.94	0.000	1.015		1.078
					259.56	0.000	1.021		1.084
					261.18	0.000	1.028		1.091
					262.73	0.000	1.034		1.096
					264.35	0.000	1.040		1.103
					265.97	0.000	1.046		1.109
					267.60	0.000	1.052		1.115
					269.14	0.000	1.059		1.121
					270.68	0.000	1.065		1.127
					272.14	0.000	1.071		1.132
					273.68	1.198	1.077		1.138
					276.77	1.210	1.083		1.150
					280.83	1.225	1.089		1.166
					284.16	1.240	1.095		1.178
					287.89	1.256	1.101		1.193
					291.22	1.267	1.106		1.206

					294.46	1.284	1.112		1.218
					297.55	1.300	1.124		1.230
					300.71	1.316	1.140		1.242
1,2-Dibenzolethylene	C16H12O2	236.27	0.127	Training set 1, Training set 2	88.80	0.464	1.152		0.428
					97.50	0.490	1.167		0.460
					107.80	0.527	1.180		0.497
					127.00	0.590	1.192		0.565
					138.60	0.628	1.204		0.606
					151.50	0.674	1.216		0.651
					165.00	0.720	0.654		0.697
					178.50	0.766	0.701		0.744
					192.50	0.820	0.750		0.793
					206.30	0.870	0.799		0.842
					230.30	0.967	0.884		0.927
					251.80	1.050	0.961		1.004
					258.50	1.075	0.985		1.028
					277.60	1.159	1.054		1.097
					284.00	1.188	1.078		1.121
					291.90	1.213	1.107		1.150

1,2-Dibenzoylethane	C16H14O2	238.28	0.134	Training set 1, Training set 2	93.20	0.481	0.426		0.469
					99.80	0.506	0.451		0.494
					107.80	0.536	0.482		0.524
					117.10	0.565	0.516		0.559
					124.00	0.590	0.542		0.584
					134.10	0.632	0.579		0.621
					145.80	0.674	0.621		0.664
					156.00	0.715	0.658		0.701
4-Propylbiphenyl-4-carbonitrite	C16H15N	221.30	0.145	Training set 1, Training set 2	50.00	0.316	0.255		0.275
					60.00	0.371	0.310		0.330
					70.00	0.420	0.359		0.379
					80.00	0.464	0.405		0.425
					90.00	0.505	0.448		0.468
					100.00	0.544	0.489		0.509
					110.00	0.582	0.529		0.549
					120.00	0.620	0.569		0.589
					130.00	0.657	0.607		0.627
					140.00	0.695	0.646		0.666
					150.00	0.733	0.684		0.704

					160.00	0.772	0.722		0.742
					170.00	0.812	0.760		0.780
					180.00	0.851	0.798		0.818
					190.00	0.891	0.836		0.856
					200.00	0.933	0.874		0.894
					210.00	0.975	0.912		0.933
					220.00	1.018	0.951		0.971
					230.00	1.062	0.989		1.009
					240.00	1.105	1.028		1.048
					250.00	1.149	1.067		1.087
					260.00	1.193	1.105		1.126
					270.00	1.238	1.145		1.165
					280.00	1.284	1.184		1.204
					290.00	1.331	1.223		1.243
					300.00	1.378	1.263		1.283
					310.00	1.425	1.303		1.323
					320.00	1.468	1.343		1.363
4-trans-4-Propylcyclhexyl	C16H21N	228.84	0.167	Training set 1, Training set 2	50.00	0.308	0.300		0.320
					60.00	0.365	0.365		0.384

benzonitrile					70.00	0.419	0.422		0.441
					80.00	0.468	0.475		0.494
					90.00	0.514	0.524		0.543
					100.00	0.557	0.571		0.590
					110.00	0.600	0.616		0.635
					120.00	0.640	0.660		0.679
					130.00	0.680	0.703		0.722
					140.00	0.719	0.745		0.765
					150.00	0.759	0.788		0.807
					160.00	0.797	0.829		0.849
					170.00	0.836	0.871		0.891
					180.00	0.876	0.913		0.932
					190.00	0.915	0.954		0.974
					200.00	0.957	0.995		1.015
					210.00	1.001	1.037		1.056
					220.00	1.048	1.078		1.098
					230.00	1.099	1.120		1.139
					240.00	1.144	1.161		1.181
					250.00	1.198	1.203		1.222

					260.00	1.255	1.245		1.264
N-(2-hydroxy-4-4methodoxybenzylidine)-p-butylaniline	C18H21NO2	283.36	0.148	Test set 1, Training set 2	50.00	0.281	0.475		0.314
					60.00	0.342	0.567		0.370
					70.00	0.399	0.647		0.420
					80.00	0.453	0.718		0.467
					90.00	0.503	0.783		0.511
					100.00	0.550	0.845		0.554
					110.00	0.596	0.262		0.595
					120.00	0.641	0.318		0.635
					130.00	0.684	0.369		0.674
					140.00	0.728	0.416		0.713
					150.00	0.772	0.460		0.752
					160.00	0.815	0.502		0.791
					170.00	0.859	0.543		0.830
					180.00	0.903	0.583		0.868
					190.00	0.949	0.623		0.907
					200.00	0.995	0.662		0.946
					210.00	1.042	0.701		0.984
					220.00	1.092	0.739		1.023

					230.00	1.142	0.778		1.062
					240.00	1.194	0.817		1.101
					250.00	1.249	0.855		1.141
					260.00	1.307	0.894		1.180
					270.00	1.367	0.933		1.220
					280.00	1.428	0.972		1.259
					290.00	1.490	1.011		1.299
					300.00	1.592	1.050		1.339
Triphenylamine	C18H15N	245.32	0.139	Training set 1, Training set 2	101.90	0.462	1.089		0.493
					126.10	0.542	1.128		0.585
					147.40	0.619	1.168		0.665
					166.70	0.684	1.208		0.736
					184.40	0.752	1.248		0.802
					201.10	0.819	1.288		0.863
					216.80	0.878	0.904		0.922
					231.70	0.938	0.960		0.978
					246.00	0.993	1.014		1.032
					259.80	1.047	1.066		1.084
					273.10	1.102	1.117		1.135

					286.00	1.158	1.167		1.185
					298.50	1.213	1.215		1.233
					310.70	1.264	1.262		1.281
					322.60	1.315	1.309		1.327
					334.30	1.361	1.355		1.373
					345.70	1.402	1.400		1.419
1,2-Diphenylbenzimidazole	C19H14N2	270.33	0.129	Training set 1, Training set 2	50.00	0.218	0.225		0.258
					100.00	0.457	0.435		0.468
					150.00	0.615	0.614		0.647
					200.00	0.789	0.791		0.823
					250.00	0.968	0.970		1.003
					298.15	1.179	1.148		1.181
					350.00	1.409	1.345		1.378
					384.90	1.563	1.481		1.514
N-benzoyl-o-aminodiphenylamine	C19H16N2O	288.35	0.132	Training set 1, Training set 2	50.00	0.230	0.230		0.278
					100.00	0.459	0.443		0.492
					150.00	0.620	0.625		0.673
					200.00	0.812	0.803		0.852
					250.00	1.025	0.985		1.034

					298.15	1.237	1.165		1.213
Triphenylcarbinol	C19H16O	260.33	0.138	Training set 1, Training set 2	101.90	0.469	0.474		0.493
					126.10	0.554	0.566		0.586
					147.40	0.628	0.645		0.665
					166.70	0.701	0.716		0.736
					184.40	0.768	0.782		0.801
					201.10	0.831	0.844		0.863
					216.80	0.890	0.902		0.922
					231.70	0.948	0.958		0.977
					246.00	1.004	1.012		1.031
					259.80	1.062	1.064		1.084
					273.10	1.119	1.115		1.134
					286.00	1.172	1.164		1.184
					298.50	1.225	1.213		1.232
					310.70	1.276	1.260		1.280
					322.60	1.324	1.307		1.326
					334.30	1.368	1.353		1.372
					345.70	1.410	1.398		1.418
N-p-	C19H23NO	281.39	0.156	Training set 1,	50.00	0.320	0.279		0.312

Ethoxydenzylidene-p-butylaniline				Training set 2	60.00	0.388	0.338		0.372
					70.00	0.463	0.392		0.425
					80.00	0.492	0.441		0.475
					90.00	0.526	0.487		0.521
					100.00	0.565	0.531		0.565
					110.00	0.603	0.574		0.608
					120.00	0.640	0.616		0.650
					130.00	0.677	0.657		0.691
					140.00	0.714	0.698		0.732
					150.00	0.751	0.738		0.772
					160.00	0.788	0.778		0.812
					170.00	0.827	0.818		0.852
					180.00	0.866	0.858		0.892
					190.00	0.907	0.898		0.932
					200.00	0.949	0.938		0.972
					210.00	0.991	0.978		1.012
					220.00	1.035	1.018		1.052
					230.00	1.082	1.058		1.092
					240.00	1.129	1.098		1.132

					250.00	1.178	1.139		1.173
					260.00	1.228	1.179		1.213
					270.00	1.281	1.220		1.254
p-Hexyloxybenzylidene-p-toluidine	C20H25NO	295.42	0.159	Training set 1, Training set 2	50.00	0.318	0.279		0.316
					60.00	0.393	0.338		0.377
					70.00	0.438	0.392		0.432
					80.00	0.488	0.441		0.482
					90.00	0.534	0.487		0.529
					100.00	0.577	0.531		0.574
					110.00	0.618	0.585		0.617
					120.00	0.657	0.627		0.659
					130.00	0.696	0.669		0.701
					140.00	0.734	0.710		0.742
					150.00	0.772	0.751		0.783
					160.00	0.809	0.791		0.824
					170.00	0.848	0.832		0.864
					180.00	0.888	0.872		0.904
					190.00	0.928	0.912		0.945
					200.00	0.969	0.953		0.985

					210.00	1.012	0.993		1.025
					220.00	1.056	1.033		1.066
					230.00	1.102	1.074		1.106
					240.00	1.150	1.115		1.147
					250.00	1.201	1.155		1.187
1,3,5-Triphenyltriazine	C21H15N3	309.37	0.126	Test set 1, Training set 2	50.00	0.232	0.242		0.262
					60.00	0.275	0.293		0.309
					80.00	0.352	0.340		0.392
					100.00	0.421	0.384		0.466
					150.00	0.582	0.425		0.641
					200.00	0.743	0.465		0.815
					250.00	0.929	0.219		0.992
					298.15	1.115	0.266		1.167
					300.00	1.122	0.348		1.173
					330.00	1.235	0.423		1.285
1,2-Dinaphtylmethane	C21H16	268.35	0.138	Training set 1, Training set 2	50.00	0.235	0.598		0.235
					60.00	0.277	0.771		0.277
					70.00	0.315	0.948		0.315
					80.00	0.349	1.123		0.349

					90.00	0.383	1.130		0.383
					100.00	0.416	1.242		0.416
					110.00	0.448	0.504		0.448
					120.00	0.481	0.541		0.481
					130.00	0.514	0.579		0.514
					140.00	0.549	0.616		0.549
					150.00	0.585	0.653		0.585
					160.00	0.619	0.690		0.619
					170.00	0.655	0.727		0.655
					180.00	0.692	0.763		0.692
					190.00	0.731	0.800		0.731
					200.00	0.768	0.837		0.768
					210.00	0.809	0.874		0.809
					220.00	0.850	0.912		0.850
					230.00	0.890	0.949		0.890
					240.00	0.930	0.987		0.930
					250.00	0.972	1.024		0.972
					260.00	1.014	1.062		1.014
					270.00	1.055	1.100		1.055

					273.15	1.068	1.112		1.068
					280.00	1.096	1.139		1.096
					290.00	1.138	1.177		1.138
					298.15	1.173	1.208		1.173
					300.00	1.181	1.216		1.181
					310.00	1.223	1.255		1.223
					320.00	1.265	1.294		1.265
					330.00	1.307	1.333		1.307
					340.00	1.348	1.372		1.348
					350.00	1.389	1.412		1.389
					360.00	1.430	1.452		1.430
					369.55	1.468	1.490		1.468
4,4-Dipjenylenephtalidodicarboxylic acid dihydrazide	C22H18N4O4	402.38	0.119	Training set 1, Training set 2	60.00	0.256	0.250		0.345
					80.00	0.347	0.328		0.423
					100.00	0.423	0.399		0.494
					120.00	0.501	0.467		0.562
					140.00	0.577	0.533		0.628
					160.00	0.652	0.600		0.695
					180.00	0.728	0.666		0.761

					200.00	0.802	0.733		0.828
					220.00	0.876	0.801		0.896
					240.00	0.945	0.869		0.964
					260.00	1.014	0.938		1.033
					280.00	1.081	1.008		1.103
					298.15	1.145	1.073		1.168
N-p-Hexyloxybenzylidene-p-butylanaline	C23H31NO	337.50	0.166	Test set 1, Training set 2	50.00	0.331	0.298		0.326
					60.00	0.397	0.362		0.390
					70.00	0.454	0.419		0.447
					80.00	0.506	0.471		0.499
					90.00	0.554	0.520		0.548
					100.00	0.599	0.566		0.594
					120.00	0.685	0.655		0.683
					140.00	0.769	0.740		0.768
					160.00	0.854	0.824		0.852
					180.00	0.940	0.906		0.935
					200.00	1.030	0.989		1.017
					220.00	1.123	1.072		1.100
					240.00	1.214	1.154		1.183

					260.00	1.311	1.237		1.266
					280.00	1.414	1.321		1.349
					298.15	1.517	1.397		1.425
					300.00	1.530	1.405		1.433
5,26:13.18-Diimino-7,11:20,24-dimethenodibenzo[c,N][1,6,12,17]tetraazacyclodocosine	C28H18N6	438.48	0.119	Test set 1, Training set 2	50.00	0.182	0.205		0.265
					100.00	0.354	0.397		0.458
					150.00	0.496	0.563		0.624
					200.00	0.657	0.729		0.790
					250.00	0.841	0.899		0.960
					298.15	1.018	1.068		1.128
					350.00	1.207	1.255		1.316
					400.00	1.420	1.442		1.503
					450.00	1.593	1.635		1.696
					500.00	1.764	1.834		1.895
1,2-bis(4-Octyloxybenzoyl)hydrazine	C30H44N2O4	496.69	0.161	Test set 1, Training set 2	50.00	0.296	0.288		0.347
					60.00	0.361	0.350		0.408
					70.00	0.421	0.405		0.464
					80.00	0.478	0.456		0.514
					90.00	0.530	0.503		0.562

					100.00	0.578	0.548		0.607
					120.00	0.660	0.635		0.694
					140.00	0.741	0.719		0.777
					160.00	0.819	0.801		0.859
					180.00	0.898	0.882		0.941
					200.00	0.981	0.963		1.022
					220.00	1.070	1.044		1.103
					240.00	1.164	1.126		1.185
					260.00	1.268	1.208		1.267
					280.00	1.394	1.290		1.349
					298.15	1.502	1.366		1.425
					300.00	1.518	1.373		1.432
					320.00	1.648	1.457		1.516
					340.00	1.788	1.541		1.600
					360.00	1.940	1.626		1.685
					380.00	2.129	1.711		1.770
Hexaphenylisomelamine	C39H30N6	582.67	0.129	Test set 1, Training set 2	50.00	0.261	0.224		0.270
					100.00	0.437	0.432		0.478
					150.00	0.598	0.610		0.656

					200.00	0.775	0.786		0.832
					250.00	0.969	0.966		1.011
					298.15	1.154	1.143		1.188
					330.00	1.272	1.263		1.308
Hexaphenylmelamine	C39H30N6	582.71	0.129	Test set 1, Training set 2	50.00	0.235	0.224		0.270
					100.00	0.419	0.432		0.478
					150.00	0.580	0.610		0.656
					200.00	0.761	0.786		0.832
					250.00	0.958	0.966		1.011
					298.15	1.143	1.143		1.188
					330.00	1.268	1.263		1.308
Benzene-hexa-nonanoate	C60H102O12	1015.46	0.171	Test set 1, Training set 2	50.00	0.339	0.309		0.369
					60.00	0.414	0.375		0.435
					70.00	0.483	0.434		0.494
					80.00	0.545	0.488		0.548
					90.00	0.601	0.538		0.598
					100.00	0.652	0.586		0.646
					120.00	0.746	0.677		0.737
					140.00	0.832	0.764		0.824

					160.00	0.915	0.849		0.909
					180.00	1.002	0.934		0.994
					200.00	1.095	1.018		1.078
					220.00	1.203	1.102		1.162
					240.00	1.359	1.186		1.246
Benzene-hexa-decanoate	C66H114O12	1099.62	0.175	Test set 1, Training set 2	50.00	0.322	0.316		0.371
					60.00	0.402	0.383		0.439
					70.00	0.475	0.443		0.499
					80.00	0.539	0.498		0.554
					90.00	0.597	0.549		0.605
					100.00	0.648	0.598		0.653
					120.00	0.742	0.690		0.746
					140.00	0.822	0.778		0.834
					160.00	0.905	0.865		0.920
					180.00	0.985	0.950		1.005
					200.00	1.067	1.035		1.090
					220.00	1.155	1.119		1.175
					240.00	1.249	1.204		1.259
					260.00	1.356	1.289		1.344

					280.00	1.488	1.374		1.429

Aromatics									
Naphtalene	C10H8	128.17	0.140	Test set 1, Training set 2	50.00	0.289	0.247	0.222	0.247
					60.00	0.333	0.300	0.268	0.300
					70.00	0.371	0.347	0.312	0.347
					80.00	0.406	0.392	0.353	0.392
					90.00	0.439	0.434	0.393	0.434
					100.00	0.471	0.474	0.431	0.474
					120.00	0.535	0.552	0.506	0.552
					140.00	0.602	0.627	0.580	0.627
					160.00	0.674	0.702	0.654	0.702
					180.00	0.751	0.777	0.728	0.777
					200.00	0.832	0.851	0.802	0.851
					220.00	0.918	0.927	0.877	0.927
					240.00	1.008	1.002	0.952	1.002
					260.00	1.102	1.079	1.028	1.079
					280.00	1.200	1.156	1.105	1.156
					298.15	1.292	1.226	1.176	1.226

					300.00	1.302	1.234	1.183	1.234
					320.00	1.412	1.312	1.261	1.312
					340.00	1.523	1.392	1.341	1.392
					353.37	1.595	1.445	1.394	1.445
1,2,3,4-Tetrahydronaphthalene	C10H12	132.20	0.166	Test set 1, Training set 2	50.00	0.312	0.299	0.258	0.299
					60.00	0.360	0.363	0.313	0.363
					70.00	0.403	0.420	0.363	0.420
					80.00	0.442	0.472	0.410	0.472
					90.00	0.480	0.521	0.456	0.521
					100.00	0.515	0.568	0.499	0.568
					110.00	0.552	0.613	0.542	0.613
					120.00	0.589	0.657	0.584	0.657
					130.00	0.627	0.700	0.626	0.700
					140.00	0.664	0.742	0.667	0.742
					150.00	0.703	0.784	0.708	0.784
					160.00	0.742	0.826	0.749	0.826
					170.00	0.782	0.868	0.790	0.868
					180.00	0.824	0.909	0.831	0.909
					190.00	0.869	0.950	0.872	0.950

					200.00	0.916	0.992	0.913	0.992
					210.00	0.968	1.033	0.954	1.033
					220.00	1.021	1.074	0.995	1.074
					230.00	1.075	1.116	1.036	1.116
					237.36	1.114	1.146	1.066	1.146
1-Methylnaphthalene	C11H10	142.20	0.148	Test set 1, Training set 2	50.00	0.289	0.261	0.232	0.261
					60.00	0.337	0.317	0.281	0.317
					70.00	0.381	0.367	0.326	0.367
					80.00	0.423	0.414	0.369	0.414
					90.00	0.463	0.458	0.411	0.458
					100.00	0.500	0.500	0.451	0.500
					110.00	0.538	0.541	0.490	0.541
					120.00	0.576	0.581	0.529	0.581
					130.00	0.615	0.620	0.567	0.620
					140.00	0.653	0.659	0.605	0.659
					150.00	0.692	0.698	0.643	0.698
					160.00	0.732	0.737	0.681	0.737
					170.00	0.772	0.775	0.719	0.775
					180.00	0.813	0.814	0.757	0.814

					190.00	0.854	0.852	0.796	0.852
					200.00	0.895	0.891	0.834	0.891
					210.00	0.937	0.930	0.872	0.930
					220.00	0.981	0.969	0.911	0.969
					230.00	1.026	1.007	0.950	1.007
					240.00	1.071	1.046	0.989	1.046
					240.79	1.074	1.050	0.992	1.050
2-Methylnaphthalene	C11H10	142.20	0.148	Test set 1, Training set 2	50.00	0.308	0.261	0.232	0.261
					60.00	0.360	0.317	0.281	0.317
					70.00	0.405	0.367	0.326	0.367
					80.00	0.446	0.414	0.369	0.414
					90.00	0.486	0.458	0.411	0.458
					100.00	0.521	0.500	0.451	0.500
					110.00	0.557	0.541	0.490	0.541
					120.00	0.592	0.581	0.529	0.581
					130.00	0.627	0.620	0.567	0.620
					140.00	0.663	0.659	0.605	0.659
					150.00	0.699	0.698	0.643	0.698
					160.00	0.735	0.737	0.681	0.737

					170.00	0.771	0.775	0.719	0.775
					180.00	0.808	0.814	0.757	0.814
					190.00	0.847	0.852	0.796	0.852
					200.00	0.885	0.891	0.834	0.891
					210.00	0.924	0.930	0.872	0.930
					220.00	0.965	0.969	0.911	0.969
					230.00	1.006	1.007	0.950	1.007
					240.00	1.047	1.046	0.989	1.046
					250.00	1.089	1.086	1.028	1.086
					260.00	1.134	1.125	1.067	1.125
					270.00	1.184	1.164	1.106	1.164
Acenaphthene	C11H10	154.21	0.148	Test set 1, Training set 2	50.00	0.260	0.261	0.232	0.261
					60.00	0.302	0.317	0.281	0.317
					70.00	0.340	0.367	0.326	0.367
					80.00	0.373	0.414	0.369	0.414
					90.00	0.409	0.458	0.411	0.458
					100.00	0.440	0.500	0.451	0.500
					110.00	0.471	0.541	0.490	0.541
					120.00	0.503	0.581	0.529	0.581

					130.00	0.537	0.620	0.567	0.620
					140.00	0.571	0.659	0.605	0.659
					150.00	0.605	0.698	0.643	0.698
					160.00	0.641	0.737	0.681	0.737
					170.00	0.677	0.775	0.719	0.775
					180.00	0.715	0.814	0.757	0.814
					190.00	0.754	0.852	0.796	0.852
					200.00	0.795	0.891	0.834	0.891
					210.00	0.835	0.930	0.872	0.930
					220.00	0.876	0.969	0.911	0.969
					230.00	0.919	1.007	0.950	1.007
					240.00	0.962	1.046	0.989	1.046
					250.00	1.007	1.086	1.028	1.086
					260.00	1.051	1.125	1.067	1.125
					270.00	1.097	1.164	1.106	1.164
					273.15	1.112	1.177	1.119	1.177
					280.00	1.144	1.204	1.146	1.204
					290.00	1.195	1.244	1.186	1.244
					298.15	1.235	1.277	1.218	1.277

					300.00	1.244	1.284	1.225	1.284
					310.00	1.295	1.324	1.266	1.324
					320.00	1.351	1.365	1.306	1.365
					330.00	1.410	1.405	1.346	1.405
					340.00	1.472	1.446	1.387	1.446
					350.00	1.548	1.487	1.428	1.487
					360.00	1.619	1.528	1.469	1.528
Biphenyl	C12H10	154.21	0.143	Test set 1, Training set 2	50.00	0.301	0.251	0.225	0.251
					60.00	0.346	0.305	0.272	0.305
					70.00	0.387	0.354	0.316	0.354
					80.00	0.423	0.399	0.358	0.399
					90.00	0.457	0.441	0.398	0.441
					100.00	0.491	0.482	0.437	0.482
					110.00	0.524	0.522	0.475	0.522
					120.00	0.557	0.561	0.513	0.561
					130.00	0.591	0.599	0.551	0.599
					140.00	0.625	0.637	0.588	0.637
					150.00	0.660	0.675	0.625	0.675
					160.00	0.696	0.713	0.662	0.713

					170.00	0.733	0.750	0.700	0.750
					180.00	0.771	0.788	0.737	0.788
					190.00	0.810	0.826	0.774	0.826
					200.00	0.850	0.864	0.812	0.864
					210.00	0.891	0.902	0.850	0.902
					220.00	0.933	0.940	0.887	0.940
					230.00	0.976	0.978	0.925	0.978
					240.00	1.019	1.016	0.964	1.016
					250.00	1.064	1.054	1.002	1.054
					260.00	1.107	1.093	1.040	1.093
					270.00	1.156	1.132	1.079	1.132
					280.00	1.202	1.171	1.118	1.171
					290.00	1.249	1.210	1.157	1.210
					298.15	1.286	1.242	1.189	1.242
					300.00	1.295	1.249	1.196	1.249
					310.00	1.345	1.289	1.236	1.289
					320.00	1.395	1.329	1.275	1.329
					330.00	1.444	1.368	1.315	1.368
					340.00	1.493	1.409	1.355	1.409

					342.10	1.503	1.417	1.364	1.417
1,8-Dimethylnaphthalene	C12H10	156.22	0.143	Test set 1, Training set 2	50.00	0.283	0.251	0.225	0.251
					60.00	0.333	0.305	0.272	0.305
					70.00	0.379	0.354	0.316	0.354
					80.00	0.422	0.399	0.358	0.399
					90.00	0.465	0.441	0.398	0.441
					100.00	0.508	0.482	0.437	0.482
					110.00	0.549	0.522	0.475	0.522
					120.00	0.593	0.561	0.513	0.561
					130.00	0.635	0.599	0.551	0.599
					140.00	0.678	0.637	0.588	0.637
					150.00	0.721	0.675	0.625	0.675
					160.00	0.765	0.713	0.662	0.713
					170.00	0.810	0.750	0.700	0.750
					180.00	0.854	0.788	0.737	0.788
					190.00	0.900	0.826	0.774	0.826
					200.00	0.948	0.864	0.812	0.864
					210.00	0.997	0.902	0.850	0.902
					220.00	1.047	0.940	0.887	0.940

					230.00	1.100	0.978	0.925	0.978
					240.00	1.155	1.016	0.964	1.016
					250.00	1.214	1.054	1.002	1.054
					260.00	1.278	1.093	1.040	1.093
2,6-Dimethylnaphthalene	C12H12	156.22	0.154	Test set 1, Training set 2	50.00	0.335	0.273	0.240	0.273
					60.00	0.387	0.331	0.291	0.331
					70.00	0.433	0.384	0.338	0.384
					80.00	0.473	0.432	0.382	0.432
					90.00	0.511	0.478	0.425	0.478
					100.00	0.548	0.522	0.466	0.522
					110.00	0.581	0.564	0.507	0.564
					120.00	0.616	0.605	0.546	0.605
					130.00	0.650	0.646	0.586	0.646
					140.00	0.685	0.686	0.625	0.686
					150.00	0.719	0.726	0.664	0.726
					160.00	0.755	0.765	0.703	0.765
					170.00	0.791	0.805	0.742	0.805
					180.00	0.828	0.844	0.781	0.844
					190.00	0.865	0.884	0.820	0.884

					200.00	0.904	0.923	0.860	0.923
					210.00	0.941	0.963	0.899	0.963
					220.00	0.981	1.002	0.938	1.002
					230.00	1.022	1.042	0.978	1.042
					240.00	1.062	1.082	1.018	1.082
					250.00	1.103	1.122	1.057	1.122
					260.00	1.142	1.162	1.097	1.162
					270.00	1.184	1.203	1.137	1.203
					273.15	1.197	1.215	1.150	1.215
					280.00	1.225	1.243	1.178	1.243
					290.00	1.269	1.284	1.218	1.284
					298.15	1.304	1.317	1.251	1.317
					300.00	1.311	1.324	1.259	1.324
					310.00	1.353	1.365	1.300	1.365
					320.00	1.397	1.406	1.341	1.406
					330.00	1.442	1.447	1.382	1.447
					340.00	1.486	1.489	1.423	1.489
					350.00	1.531	1.530	1.465	1.530
					360.00	1.577	1.572	1.506	1.572

					370.00	1.622	1.614	1.548	1.614
					380.00	1.676	1.656	1.590	1.656
					383.32	1.691	1.670	1.604	1.670
2,7-Dimethylnaphtalene	C12H12	156.22	0.154	Test set 1, Training set 2	50.00	0.335	0.273	0.240	0.273
					60.00	0.386	0.331	0.291	0.331
					70.00	0.427	0.384	0.338	0.384
					80.00	0.466	0.432	0.382	0.432
					90.00	0.505	0.478	0.425	0.478
					100.00	0.540	0.522	0.466	0.522
					110.00	0.575	0.564	0.507	0.564
					120.00	0.610	0.605	0.546	0.605
					130.00	0.645	0.646	0.586	0.646
					140.00	0.681	0.686	0.625	0.686
					150.00	0.717	0.726	0.664	0.726
					160.00	0.754	0.765	0.703	0.765
					170.00	0.790	0.805	0.742	0.805
					180.00	0.827	0.844	0.781	0.844
					190.00	0.865	0.884	0.820	0.884
					200.00	0.903	0.923	0.860	0.923

					210.00	0.941	0.963	0.899	0.963
					220.00	0.982	1.002	0.938	1.002
					230.00	1.022	1.042	0.978	1.042
					240.00	1.061	1.082	1.018	1.082
					250.00	1.104	1.122	1.057	1.122
					260.00	1.146	1.162	1.097	1.162
					270.00	1.188	1.203	1.137	1.203
					273.15	1.202	1.215	1.150	1.215
					280.00	1.231	1.243	1.178	1.243
					290.00	1.274	1.284	1.218	1.284
					298.15	1.309	1.317	1.251	1.317
					300.00	1.316	1.324	1.259	1.324
					310.00	1.361	1.365	1.300	1.365
					320.00	1.405	1.406	1.341	1.406
					330.00	1.449	1.447	1.382	1.447
					340.00	1.486	1.489	1.423	1.489
					350.00	1.538	1.530	1.465	1.530
					360.00	1.585	1.572	1.506	1.572
					368.81	1.626	1.609	1.543	1.609

2,3-Dimethylnaphthalene	C12H12	156.22	0.154	Test set 1, Training set 2	50.00	0.282	0.273	0.240	0.273
					60.00	0.337	0.331	0.291	0.331
					70.00	0.386	0.384	0.338	0.384
					80.00	0.434	0.432	0.382	0.432
					90.00	0.483	0.478	0.425	0.478
					100.00	0.528	0.522	0.466	0.522
					110.00	0.572	0.564	0.507	0.564
					120.00	0.616	0.605	0.546	0.605
					130.00	0.660	0.646	0.586	0.646
					140.00	0.705	0.686	0.625	0.686
					150.00	0.747	0.726	0.664	0.726
					160.00	0.791	0.765	0.703	0.765
					170.00	0.834	0.805	0.742	0.805
					180.00	0.878	0.844	0.781	0.844
					190.00	0.921	0.884	0.820	0.884
					200.00	0.964	0.923	0.860	0.923
					210.00	1.012	0.963	0.899	0.963
					220.00	1.063	1.002	0.938	1.002
					226.00	1.093	1.026	0.962	1.026

Fluorene	C13H10	166.22	0.138	Test set 1, Training set 2	50.00	0.272	0.243	0.219	0.243
					60.00	0.311	0.295	0.265	0.295
					70.00	0.346	0.342	0.308	0.342
					80.00	0.379	0.385	0.348	0.385
					90.00	0.411	0.427	0.388	0.427
					100.00	0.443	0.467	0.426	0.467
					110.00	0.472	0.505	0.463	0.505
					120.00	0.504	0.543	0.500	0.543
					130.00	0.535	0.581	0.537	0.581
					140.00	0.567	0.618	0.573	0.618
					150.00	0.601	0.655	0.610	0.655
					160.00	0.636	0.692	0.646	0.692
					170.00	0.671	0.729	0.683	0.729
					180.00	0.707	0.766	0.719	0.766
					190.00	0.744	0.803	0.756	0.803
					200.00	0.782	0.840	0.793	0.840
					210.00	0.822	0.877	0.830	0.877
					220.00	0.862	0.915	0.867	0.915
					230.00	0.901	0.952	0.904	0.952

					240.00	0.942	0.990	0.942	0.990
					250.00	0.984	1.027	0.979	1.027
					260.00	1.026	1.065	1.017	1.065
					270.00	1.068	1.104	1.055	1.104
					273.15	1.082	1.116	1.067	1.116
					280.00	1.112	1.142	1.093	1.142
					288.00	1.145	1.173	1.124	1.173
Diphenylmethane	C13H12	168.24	0.149	Test set 1, Training set 2	101.90	0.525	0.511	0.461	0.511
					126.10	0.607	0.609	0.555	0.609
					147.40	0.679	0.692	0.637	0.692
					166.70	0.756	0.767	0.710	0.767
					184.40	0.826	0.836	0.778	0.836
					201.10	0.900	0.900	0.842	0.900
					216.80	0.977	0.961	0.903	0.961
					231.70	1.037	1.019	0.961	1.019
					246.00	1.102	1.076	1.017	1.076
					259.80	1.171	1.130	1.071	1.130
					273.10	1.241	1.183	1.123	1.183
					286.00	1.311	1.234	1.175	1.234

					298.50	1.388	1.284	1.225	1.284
9,10-Dihydrophenanthrene	C14H12	180.25	0.144	Training set 1, Training set 2	50.00	0.263	0.254	0.227	0.254
					60.00	0.302	0.309	0.275	0.309
					70.00	0.341	0.358	0.319	0.358
					80.00	0.374	0.403	0.362	0.403
					90.00	0.408	0.446	0.402	0.446
					100.00	0.442	0.488	0.441	0.488
					110.00	0.475	0.528	0.480	0.528
					120.00	0.508	0.567	0.518	0.567
					130.00	0.543	0.606	0.556	0.606
					140.00	0.579	0.644	0.593	0.644
					150.00	0.615	0.682	0.631	0.682
					160.00	0.653	0.720	0.668	0.720
					170.00	0.691	0.758	0.706	0.758
					180.00	0.730	0.796	0.743	0.796
					190.00	0.770	0.834	0.781	0.834
					200.00	0.812	0.872	0.819	0.872
					210.00	0.856	0.910	0.857	0.910
					220.00	0.899	0.949	0.895	0.949

					230.00	0.947	0.987	0.933	0.987
					240.00	0.995	1.026	0.971	1.026
					250.00	1.047	1.064	1.010	1.064
					260.00	1.103	1.103	1.049	1.103
Anthracene	C14H10	178.23	0.135	Training set 1, Training set 2	50.00	0.237	0.236	0.213	0.236
					60.00	0.277	0.286	0.258	0.286
					70.00	0.313	0.332	0.300	0.332
					80.00	0.347	0.374	0.340	0.374
					90.00	0.380	0.415	0.378	0.415
					100.00	0.412	0.453	0.415	0.453
					110.00	0.444	0.491	0.452	0.491
					120.00	0.477	0.529	0.488	0.529
					130.00	0.510	0.565	0.524	0.565
					140.00	0.545	0.602	0.560	0.602
					150.00	0.580	0.638	0.596	0.638
					160.00	0.616	0.674	0.632	0.674
					170.00	0.653	0.710	0.667	0.710
					180.00	0.690	0.747	0.703	0.747
					190.00	0.728	0.783	0.739	0.783

					200.00	0.767	0.819	0.776	0.819
					210.00	0.807	0.856	0.812	0.856
					220.00	0.848	0.893	0.849	0.893
					230.00	0.889	0.930	0.885	0.930
					240.00	0.931	0.967	0.922	0.967
					250.00	0.972	1.004	0.959	1.004
					260.00	1.014	1.041	0.997	1.041
					270.00	1.057	1.079	1.034	1.079
					273.15	1.070	1.091	1.046	1.091
					280.00	1.100	1.117	1.072	1.117
					290.00	1.145	1.154	1.110	1.154
					298.15	1.181	1.186	1.141	1.186
					300.00	1.189	1.193	1.148	1.193
					310.00	1.234	1.231	1.186	1.231
					320.00	1.278	1.270	1.225	1.270
					330.00	1.321	1.308	1.263	1.308
					340.00	1.364	1.347	1.302	1.347
					350.00	1.406	1.387	1.342	1.387
					400.00	1.616	1.586	1.541	1.586

					450.00	1.834	1.791	1.746	1.791
					488.93	2.027	1.955	1.909	1.955
Phenanthrene	C14H10	178.24	0.135	Training set 1, Training set 2	50.00	0.252	0.236	0.213	0.236
					60.00	0.291	0.286	0.258	0.286
					70.00	0.324	0.332	0.300	0.332
					80.00	0.357	0.374	0.340	0.374
					90.00	0.388	0.415	0.378	0.415
					100.00	0.419	0.453	0.415	0.453
					110.00	0.450	0.491	0.452	0.491
					120.00	0.483	0.529	0.488	0.529
					130.00	0.516	0.565	0.524	0.565
					140.00	0.549	0.602	0.560	0.602
					150.00	0.583	0.638	0.596	0.638
					160.00	0.618	0.674	0.632	0.674
					170.00	0.655	0.710	0.667	0.710
					180.00	0.693	0.747	0.703	0.747
					190.00	0.731	0.783	0.739	0.783
					200.00	0.770	0.819	0.776	0.819
					210.00	0.810	0.856	0.812	0.856

					220.00	0.851	0.893	0.849	0.893
					230.00	0.892	0.930	0.885	0.930
					240.00	0.933	0.967	0.922	0.967
					250.00	0.975	1.004	0.959	1.004
					260.00	1.017	1.041	0.997	1.041
					270.00	1.065	1.079	1.034	1.079
Diphenymethyne	C14H10	178.23	0.135	Training set 1, Training set 2	101.90	0.509	0.461	0.422	0.461
					126.10	0.582	0.551	0.510	0.551
					147.40	0.657	0.629	0.587	0.629
					166.70	0.735	0.698	0.656	0.698
					184.40	0.805	0.763	0.719	0.763
					201.10	0.873	0.823	0.780	0.823
					216.80	0.932	0.881	0.837	0.881
					231.70	0.991	0.936	0.892	0.936
					246.00	1.045	0.989	0.944	0.989
					259.80	1.103	1.040	0.996	1.040
					273.10	1.155	1.090	1.046	1.090
					286.00	1.211	1.139	1.094	1.139
					298.50	1.268	1.187	1.142	1.187

					310.70	1.324	1.234	1.189	1.234
					322.60	1.373	1.280	1.235	1.280
1,1-Diphenylethylene	C14H12	180.25	0.144	Training set 1, Training set 2	101.90	0.518	0.495	0.449	0.495
					126.10	0.610	0.591	0.541	0.591
					147.40	0.692	0.672	0.621	0.672
					166.70	0.773	0.746	0.693	0.746
					184.40	0.850	0.813	0.760	0.813
					201.10	0.915	0.876	0.823	0.876
					216.80	0.980	0.936	0.883	0.936
					231.70	1.042	0.994	0.940	0.994
					246.00	1.107	1.049	0.995	1.049
					259.80	1.177	1.102	1.048	1.102
1,2-Diphenylethylene	C14H12	180.25	0.144	Training set 1, Training set 2	101.90	0.506	0.495	0.449	0.495
					126.10	0.590	0.591	0.541	0.591
					147.40	0.669	0.672	0.621	0.672
					166.70	0.743	0.746	0.693	0.746
					184.40	0.815	0.813	0.760	0.813
					201.10	0.884	0.876	0.823	0.876
					216.80	0.947	0.936	0.883	0.936

					231.70	1.000	0.994	0.940	0.994
					246.00	1.058	1.049	0.995	1.049
					259.80	1.117	1.102	1.048	1.102
					273.10	1.179	1.154	1.100	1.154
					286.00	1.233	1.205	1.150	1.205
					298.50	1.291	1.254	1.200	1.254
					310.70	1.349	1.303	1.248	1.303
					322.30	1.400	1.349	1.294	1.349
					334.30	1.453	1.397	1.342	1.397
					345.70	1.497	1.444	1.388	1.444
trans-Stillbene	C14H12	180.25	0.144	Training set 1, Training set 2	50.00	0.305	0.254	0.227	0.254
					60.00	0.354	0.309	0.275	0.309
					70.00	0.398	0.358	0.319	0.358
					80.00	0.435	0.403	0.362	0.403
					90.00	0.471	0.446	0.402	0.446
					100.00	0.505	0.488	0.441	0.488
					110.00	0.539	0.528	0.480	0.528
					120.00	0.572	0.567	0.518	0.567
					130.00	0.605	0.606	0.556	0.606

					140.00	0.639	0.644	0.593	0.644
					150.00	0.673	0.682	0.631	0.682
					160.00	0.708	0.720	0.668	0.720
					170.00	0.750	0.758	0.706	0.758
					180.00	0.792	0.796	0.743	0.796
					190.00	0.830	0.834	0.781	0.834
					200.00	0.870	0.872	0.819	0.872
					210.00	0.910	0.910	0.857	0.910
					220.00	0.953	0.949	0.895	0.949
					230.00	0.994	0.987	0.933	0.987
					240.00	1.038	1.026	0.971	1.026
					250.00	1.081	1.064	1.010	1.064
					260.00	1.124	1.103	1.049	1.103
					270.00	1.168	1.142	1.088	1.142
					280.00	1.216	1.181	1.127	1.181
					290.00	1.262	1.221	1.166	1.221
					298.15	1.304	1.253	1.198	1.253
					300.00	1.313	1.260	1.205	1.260
					310.00	1.351	1.300	1.245	1.300

					320.00	1.398	1.340	1.285	1.340
					330.00	1.443	1.380	1.325	1.380
					340.00	1.489	1.420	1.365	1.420
1,1-Diphenylethane	C14H14	182.26	0.154	Training set 1, Training set 2	101.90	0.526	0.530	0.474	0.530
					126.10	0.608	0.630	0.570	0.630
					147.40	0.679	0.715	0.654	0.715
					166.70	0.751	0.792	0.729	0.792
					184.40	0.813	0.862	0.798	0.862
					201.10	0.888	0.928	0.864	0.928
					216.80	0.960	0.990	0.926	0.990
					231.70	1.028	1.049	0.984	1.049
1,2-Diphenylethane	C14H14	182.26	0.154	Training set 1, Training set 2	50.00	0.327	0.273	0.240	0.273
					60.00	0.379	0.331	0.291	0.331
					70.00	0.422	0.384	0.338	0.384
					80.00	0.460	0.432	0.382	0.432
					90.00	0.495	0.478	0.425	0.478
					100.00	0.528	0.522	0.466	0.522
					110.00	0.561	0.564	0.507	0.564
					120.00	0.594	0.605	0.546	0.605

					130.00	0.629	0.646	0.586	0.646
					140.00	0.663	0.686	0.625	0.686
					150.00	0.699	0.726	0.664	0.726
					160.00	0.736	0.765	0.703	0.765
					170.00	0.771	0.805	0.742	0.805
					180.00	0.809	0.844	0.781	0.844
					190.00	0.847	0.884	0.820	0.884
					200.00	0.887	0.923	0.859	0.923
					210.00	0.930	0.963	0.899	0.963
					220.00	0.970	1.002	0.938	1.002
					230.00	1.012	1.042	0.978	1.042
					240.00	1.057	1.082	1.017	1.082
					250.00	1.102	1.122	1.057	1.122
					260.00	1.153	1.162	1.097	1.162
4-Methylphenanthrene	C15H12	192.26	0.140	Training set 1, Training set 2	50.00	0.253	0.247	0.222	0.247
					60.00	0.291	0.300	0.268	0.300
					70.00	0.326	0.347	0.312	0.347
					80.00	0.361	0.392	0.353	0.392
					90.00	0.396	0.434	0.393	0.434

					100.00	0.430	0.474	0.431	0.474
					110.00	0.466	0.513	0.469	0.513
					120.00	0.501	0.552	0.506	0.552
					130.00	0.538	0.590	0.543	0.590
					140.00	0.575	0.627	0.580	0.627
					150.00	0.614	0.665	0.617	0.665
					160.00	0.656	0.702	0.654	0.702
					170.00	0.704	0.739	0.691	0.739
					180.00	0.764	0.777	0.728	0.777
					182.00	0.778	0.784	0.735	0.784
Fluoranthene	C16H10	202.26	0.129	Training set 1, Training set 2	50.00	0.229	0.224	0.204	0.224
					60.00	0.266	0.271	0.247	0.271
					70.00	0.301	0.315	0.288	0.315
					80.00	0.333	0.356	0.326	0.356
					90.00	0.365	0.394	0.363	0.394
					100.00	0.395	0.432	0.399	0.432
					110.00	0.426	0.468	0.434	0.468
					120.00	0.458	0.504	0.469	0.504
					130.00	0.490	0.539	0.504	0.539

					140.00	0.524	0.575	0.538	0.575
					150.00	0.559	0.610	0.573	0.610
					160.00	0.594	0.645	0.608	0.645
					170.00	0.629	0.680	0.642	0.680
					180.00	0.666	0.715	0.677	0.715
					190.00	0.703	0.750	0.712	0.750
					200.00	0.741	0.785	0.747	0.785
					210.00	0.780	0.821	0.783	0.821
					220.00	0.820	0.857	0.818	0.857
					230.00	0.860	0.892	0.854	0.892
					240.00	0.900	0.928	0.890	0.928
					250.00	0.941	0.964	0.926	0.964
					260.00	0.981	1.001	0.962	1.001
					270.00	1.022	1.037	0.999	1.037
					273.15	1.035	1.049	1.010	1.049
					280.00	1.063	1.074	1.035	1.074
					290.00	1.104	1.111	1.072	1.111
					298.15	1.138	1.141	1.102	1.141
					300.00	1.146	1.148	1.109	1.148

					310.00	1.188	1.186	1.147	1.186
					320.00	1.229	1.223	1.184	1.223
					330.00	1.271	1.261	1.222	1.261
					340.00	1.312	1.299	1.260	1.299
					350.00	1.352	1.338	1.298	1.338
					360.00	1.393	1.376	1.337	1.376
					370.00	1.435	1.415	1.376	1.415
					380.00	1.477	1.454	1.415	1.454
					383.36	1.491	1.467	1.428	1.467
4,5,9,10-Tetrahydropyrene	C16H14	206.29	0.145	Training set 1, Training set 2	50.00	0.220	0.257	0.229	0.257
					60.00	0.258	0.312	0.277	0.312
					70.00	0.293	0.361	0.322	0.361
					80.00	0.327	0.407	0.364	0.407
					90.00	0.361	0.450	0.405	0.450
					100.00	0.395	0.492	0.444	0.492
					120.00	0.464	0.572	0.522	0.572
					140.00	0.535	0.649	0.597	0.649
					160.00	0.610	0.726	0.673	0.726
					180.00	0.687	0.802	0.748	0.802

					200.00	0.767	0.879	0.824	0.879
					220.00	0.850	0.956	0.900	0.956
					240.00	0.936	1.033	0.977	1.033
					260.00	1.026	1.111	1.055	1.111
					280.00	1.118	1.189	1.133	1.189
1,2,3,6,7,8-Hexahydropyrene	C16H16	208.30	0.154	Training set 1, Training set 2	50.00	0.215	0.273	0.240	0.273
					60.00	0.256	0.331	0.291	0.331
					70.00	0.294	0.384	0.338	0.384
					80.00	0.330	0.432	0.382	0.432
					90.00	0.366	0.478	0.425	0.478
					100.00	0.401	0.522	0.466	0.522
					120.00	0.474	0.605	0.546	0.605
					140.00	0.547	0.686	0.625	0.686
					160.00	0.623	0.765	0.703	0.765
					180.00	0.700	0.844	0.781	0.844
					200.00	0.781	0.923	0.859	0.923
					220.00	0.864	1.002	0.938	1.002
					240.00	0.952	1.082	1.017	1.082
					260.00	1.043	1.162	1.097	1.162

					280.00	1.137	1.243	1.178	1.243
					298.15	1.227	1.317	1.251	1.317
					300.00	1.236	1.324	1.259	1.324
					320.00	1.339	1.406	1.341	1.406
					340.00	1.446	1.489	1.423	1.489
					360.00	1.559	1.572	1.506	1.572
					370.00	1.619	1.614	1.548	1.614
Triphenylene	C18H12	228.28	0.131	Training set 1, Training set 2	50.00	0.222	0.229	0.208	0.229
					60.00	0.261	0.278	0.252	0.278
					70.00	0.296	0.323	0.294	0.323
					80.00	0.329	0.364	0.333	0.364
					90.00	0.361	0.404	0.370	0.404
					100.00	0.393	0.442	0.407	0.442
					110.00	0.425	0.479	0.443	0.479
					120.00	0.457	0.515	0.478	0.515
					130.00	0.490	0.552	0.513	0.552
					140.00	0.524	0.587	0.549	0.587
					150.00	0.559	0.623	0.584	0.623
					160.00	0.594	0.659	0.619	0.659

					170.00	0.630	0.694	0.654	0.694
					180.00	0.667	0.730	0.690	0.730
					190.00	0.705	0.766	0.725	0.766
					200.00	0.742	0.801	0.761	0.801
					210.00	0.781	0.837	0.797	0.837
					220.00	0.819	0.874	0.833	0.874
					230.00	0.859	0.910	0.869	0.910
					240.00	0.899	0.946	0.905	0.946
					250.00	0.940	0.983	0.942	0.983
					260.00	0.981	1.020	0.978	1.020
					270.00	1.021	1.057	1.015	1.057
					273.15	1.034	1.069	1.027	1.069
					280.00	1.062	1.094	1.052	1.094
					290.00	1.103	1.132	1.090	1.132
					298.15	1.135	1.162	1.120	1.162
					300.00	1.143	1.169	1.127	1.169
					310.00	1.183	1.207	1.165	1.207
					320.00	1.223	1.245	1.203	1.245
					330.00	1.263	1.284	1.242	1.284

					340.00	1.303	1.322	1.280	1.322
					350.00	1.342	1.361	1.319	1.361
					360.00	1.381	1.400	1.358	1.400
					370.00	1.418	1.439	1.397	1.439
					380.00	1.454	1.478	1.436	1.478
					390.00	1.490	1.518	1.476	1.518
					400.00	1.526	1.558	1.516	1.558
					410.00	1.563	1.598	1.556	1.598
					420.00	1.599	1.638	1.596	1.638
					430.00	1.633	1.679	1.637	1.679
					440.00	1.666	1.720	1.678	1.720
					450.00	1.699	1.761	1.719	1.761
					460.00	1.733	1.802	1.760	1.802
					470.00	1.768	1.844	1.801	1.844
					471.01	1.771	1.848	1.805	1.848
o-Terphenyl	C18H14	230.31	0.139	Training set 1, Training set 2	50.00	0.276	0.244	0.219	0.244
					60.00	0.320	0.296	0.266	0.296
					70.00	0.358	0.343	0.309	0.343
					80.00	0.393	0.387	0.350	0.387

					90.00	0.426	0.429	0.389	0.429
					100.00	0.457	0.469	0.427	0.469
					110.00	0.489	0.508	0.465	0.508
					120.00	0.520	0.546	0.502	0.546
					130.00	0.551	0.583	0.538	0.583
					140.00	0.583	0.621	0.575	0.621
					150.00	0.616	0.658	0.612	0.658
					160.00	0.649	0.695	0.648	0.695
					170.00	0.684	0.732	0.685	0.732
					180.00	0.720	0.769	0.721	0.769
					190.00	0.756	0.806	0.758	0.806
					200.00	0.794	0.843	0.795	0.843
					210.00	0.832	0.880	0.832	0.880
					220.00	0.871	0.918	0.869	0.918
					230.00	0.911	0.955	0.907	0.955
					240.00	0.951	0.993	0.944	0.993
					250.00	0.992	1.031	0.982	1.031
					260.00	1.033	1.069	1.020	1.069
					270.00	1.075	1.107	1.058	1.107

					280.00	1.117	1.146	1.097	1.146
					290.00	1.159	1.184	1.135	1.184
					300.00	1.201	1.223	1.174	1.223
					310.00	1.242	1.262	1.213	1.262
					320.00	1.284	1.301	1.252	1.301
					273.15	1.088	1.119	1.070	1.119
					298.15	1.193	1.216	1.167	1.216
p-Terphenyl	C18H14	230.30	0.139	Training set 1, Training set 2	50.00	0.260	0.244	0.219	0.244
					60.00	0.306	0.296	0.266	0.296
					70.00	0.345	0.343	0.309	0.343
					80.00	0.381	0.387	0.350	0.387
					90.00	0.415	0.429	0.389	0.429
					100.00	0.449	0.469	0.427	0.469
					110.00	0.482	0.508	0.465	0.508
					120.00	0.516	0.546	0.502	0.546
					130.00	0.550	0.583	0.538	0.583
					140.00	0.586	0.621	0.575	0.621
					150.00	0.624	0.658	0.612	0.658
					160.00	0.664	0.695	0.648	0.695

					170.00	0.708	0.732	0.685	0.732
Triphenymethane	C19H16	244.34	0.143	Training set 1, Training set 2	101.90	0.476	0.492	0.446	0.492
					126.10	0.548	0.587	0.538	0.587
					147.40	0.616	0.668	0.618	0.668
					166.70	0.680	0.741	0.690	0.741
					184.40	0.743	0.808	0.756	0.808
					201.10	0.807	0.871	0.819	0.871
					216.80	0.866	0.931	0.878	0.931
					231.70	0.923	0.988	0.935	0.988
					246.00	0.979	1.043	0.989	1.043
					259.80	1.034	1.096	1.043	1.096
					273.10	1.093	1.148	1.094	1.148
					286.00	1.147	1.198	1.145	1.198
					298.50	1.209	1.247	1.194	1.247
					310.70	1.271	1.296	1.242	1.296
					322.60	1.325	1.343	1.289	1.343
					334.30	1.375	1.390	1.336	1.390
					345.70	1.416	1.436	1.382	1.436
Perylene	C20H12	252.32	0.195	Training set 1,	50.00	0.199	0.358	0.297	0.358

				Training set 2	60.00	0.234	0.435	0.360	0.435
					70.00	0.267	0.502	0.417	0.502
					80.00	0.299	0.563	0.470	0.563
					90.00	0.330	0.619	0.521	0.619
					100.00	0.361	0.673	0.569	0.673
					110.00	0.392	0.723	0.617	0.723
					120.00	0.424	0.773	0.663	0.773
					130.00	0.457	0.820	0.709	0.820
					140.00	0.490	0.867	0.754	0.867
					150.00	0.524	0.914	0.799	0.914
					160.00	0.560	0.959	0.843	0.959
					170.00	0.596	1.004	0.888	1.004
					180.00	0.632	1.049	0.932	1.049
					190.00	0.669	1.094	0.976	1.094
					200.00	0.707	1.139	1.020	1.139
					210.00	0.744	1.183	1.064	1.183
					220.00	0.782	1.227	1.107	1.227
					230.00	0.821	1.271	1.151	1.271
					240.00	0.860	1.315	1.195	1.315

					250.00	0.899	1.359	1.238	1.359
					260.00	0.939	1.403	1.282	1.403
					270.00	0.979	1.447	1.326	1.447
					273.15	0.991	1.461	1.340	1.461
					280.00	1.019	1.491	1.369	1.491
					290.00	1.058	1.535	1.413	1.535
					298.15	1.090	1.571	1.449	1.571
					300.00	1.097	1.579	1.457	1.579
					310.00	1.135	1.623	1.501	1.623
					320.00	1.173	1.667	1.544	1.667
					330.00	1.210	1.711	1.588	1.711
					340.00	1.247	1.755	1.632	1.755
					350.00	1.284	1.799	1.676	1.799
					360.00	1.320	1.842	1.720	1.842
					370.00	1.357	1.886	1.764	1.886
					380.00	1.392	1.930	1.807	1.930
					390.00	1.427	1.975	1.851	1.975
					400.00	1.462	2.019	1.895	2.019
					410.00	1.496	2.063	1.939	2.063

					420.00	1.530	2.107	1.983	2.107
					430.00	1.564	2.151	2.028	2.151
					440.00	1.598	2.195	2.072	2.195
					450.00	1.632	2.239	2.116	2.239
Triptycene	C20H14	254.33	0.134	Training set 1, Training set 2	50.00	0.217	0.234	0.212	0.234
					60.00	0.253	0.284	0.257	0.284
					70.00	0.287	0.329	0.298	0.329
					80.00	0.318	0.371	0.338	0.371
					90.00	0.348	0.411	0.376	0.411
					100.00	0.378	0.450	0.413	0.450
					110.00	0.408	0.488	0.449	0.488
					120.00	0.439	0.525	0.485	0.525
					130.00	0.470	0.561	0.521	0.561
					140.00	0.503	0.597	0.557	0.597
					150.00	0.536	0.634	0.592	0.634
					160.00	0.570	0.670	0.628	0.670
					170.00	0.605	0.706	0.664	0.706
					180.00	0.640	0.742	0.699	0.742
					190.00	0.676	0.778	0.735	0.778

					200.00	0.713	0.814	0.771	0.814
					210.00	0.751	0.850	0.807	0.850
					220.00	0.790	0.887	0.844	0.887
					230.00	0.829	0.924	0.880	0.924
					240.00	0.869	0.961	0.917	0.961
					250.00	0.910	0.998	0.954	0.998
					260.00	0.951	1.035	0.991	1.035
					270.00	0.992	1.072	1.028	1.072
					273.15	1.006	1.084	1.040	1.084
					280.00	1.034	1.110	1.066	1.110
					290.00	1.077	1.148	1.104	1.148
					298.15	1.111	1.179	1.135	1.179
					300.00	1.119	1.186	1.142	1.186
					310.00	1.161	1.224	1.180	1.224
					320.00	1.204	1.262	1.218	1.262
					330.00	1.245	1.301	1.257	1.301
					340.00	1.286	1.340	1.296	1.340
					350.00	1.327	1.379	1.335	1.379
					400.00	1.522	1.578	1.533	1.578

					450.00	1.708	1.782	1.738	1.782
					500.00	1.875	1.992	1.948	1.992
					527.18	1.964	2.109	2.064	2.109
1,1,2-Ttriphenylethylene	C20H16	256.35	0.140	Training set 1, Training set 2	101.90	0.475	0.482	0.438	0.482
					126.10	0.553	0.575	0.529	0.575
					147.40	0.622	0.655	0.607	0.655
					166.70	0.690	0.727	0.679	0.727
					184.40	0.757	0.793	0.744	0.793
					201.10	0.824	0.856	0.806	0.856
					216.80	0.890	0.915	0.865	0.915
					231.70	0.935	0.971	0.921	0.971
					246.00	0.989	1.025	0.975	1.025
					259.80	1.043	1.078	1.028	1.078
					273.10	1.098	1.129	1.079	1.129
					286.00	1.149	1.179	1.128	1.179
					298.50	1.206	1.228	1.177	1.228
					310.70	1.265	1.276	1.225	1.276
					322.30	1.317	1.321	1.271	1.321
1,1,2-Triphenylethane	C20H18	258.36	0.147	Training set 1,	101.90	0.470	0.506	0.456	0.506

				Training set 2	126.10	0.554	0.603	0.550	0.603
					147.40	0.632	0.685	0.631	0.685
					166.70	0.701	0.760	0.704	0.760
					184.40	0.772	0.828	0.772	0.828
					201.10	0.832	0.892	0.836	0.892
					216.80	0.892	0.953	0.896	0.953
					231.70	0.951	1.010	0.953	1.010
					246.00	1.009	1.066	1.009	1.066
					259.80	1.066	1.120	1.063	1.120
					273.10	1.121	1.173	1.115	1.173
					286.00	1.177	1.224	1.166	1.224
					298.50	1.237	1.274	1.216	1.274
					310.70	1.299	1.323	1.265	1.323
1,1,1-Triphenylethane	C20H18	258.36	0.147	Training set 1, Training set 2	101.90	0.468	0.506	0.456	0.506
					126.10	0.544	0.603	0.550	0.603
					147.40	0.620	0.685	0.631	0.685
					166.70	0.687	0.760	0.704	0.760
					184.40	0.755	0.828	0.772	0.828
					201.10	0.821	0.892	0.836	0.892

					216.80	0.884	0.953	0.896	0.953
					231.70	0.941	1.010	0.953	1.010
					246.00	1.001	1.066	1.009	1.066
					259.80	1.059	1.120	1.063	1.120
					273.10	1.117	1.173	1.115	1.173
					286.00	1.169	1.224	1.166	1.224
					298.50	1.226	1.274	1.216	1.274
					310.70	1.278	1.323	1.265	1.323
					322.60	1.325	1.371	1.313	1.371
					334.30	1.372	1.418	1.360	1.418
					345.70	1.420	1.465	1.406	1.465
Coronene	C24H12	300.36	0.120	Test set 1, Training set 2	50.00	0.162	0.207	0.191	0.207
					60.00	0.191	0.251	0.232	0.251
					70.00	0.218	0.292	0.270	0.292
					80.00	0.246	0.330	0.306	0.330
					90.00	0.275	0.366	0.341	0.366
					100.00	0.305	0.401	0.375	0.401
					110.00	0.337	0.435	0.408	0.435
					120.00	0.370	0.469	0.441	0.469

					130.00	0.403	0.503	0.474	0.503
					140.00	0.437	0.536	0.507	0.536
					150.00	0.471	0.569	0.540	0.569
					160.00	0.507	0.603	0.573	0.603
					170.00	0.544	0.636	0.606	0.636
					180.00	0.582	0.669	0.639	0.669
					190.00	0.619	0.703	0.672	0.703
					200.00	0.655	0.736	0.706	0.736
					210.00	0.693	0.770	0.740	0.770
p-Quaterphenyl	C24H18	306.41	0.137	Test set 1, Training set 2	50.00	0.242	0.240	0.217	0.240
					60.00	0.286	0.292	0.262	0.292
					70.00	0.325	0.338	0.305	0.338
					80.00	0.361	0.382	0.345	0.382
					90.00	0.394	0.423	0.384	0.423
					100.00	0.425	0.462	0.422	0.462
					110.00	0.459	0.501	0.459	0.501
					120.00	0.492	0.538	0.496	0.538
					130.00	0.526	0.575	0.532	0.575
					140.00	0.561	0.612	0.569	0.612

					150.00	0.597	0.649	0.605	0.649
					160.00	0.634	0.686	0.641	0.686
					170.00	0.673	0.723	0.677	0.723
					180.00	0.713	0.759	0.714	0.759
					190.00	0.755	0.796	0.750	0.796
					200.00	0.799	0.833	0.787	0.833
					210.00	0.845	0.870	0.824	0.870
					220.00	0.897	0.907	0.860	0.907
1,3,5-Triphenylbenzene	C24H18	306.38	0.137	Training set 1, Training set 2	50.00	0.259	0.240	0.2166	0.240
					60.00	0.297	0.292	0.2624	0.292
					80.00	0.377	0.382	0.3454	0.382
					100.00	0.441	0.462	0.422	0.462
					150.00	0.603	0.649	0.6047	0.649
					200.00	0.785	0.833	0.7867	0.833
					250.00	0.989	1.019	0.9722	1.019
					298.15	1.178	1.203	1.1554	1.203
					350.00	1.384	1.406	1.3581	1.406
					400.00	1.575	1.607	1.559	1.607
					446.00	1.782	1.797	1.7487	1.797

Tetraphenylmethane	C25H20	320.43	0.140	Test set 1, Training set 2	101.90	0.443	0.481621322	0.438	0.482
					126.10	0.514	0.574958856	0.529	0.575
					147.40	0.584	0.655033424	0.608	0.655
					166.70	0.648	0.727033119	0.679	0.727
					184.40	0.714	0.793039419	0.744	0.793
					201.10	0.772	0.855504127	0.806	0.856
					216.80	0.823	0.914504847	0.865	0.915
					231.70	0.884	0.970810277	0.921	0.971
					246.00	0.932	1.025172415	0.975	1.025
					259.80	0.985	1.077960319	1.028	1.078
					273.10	1.043	1.12915649	1.079	1.129
					286.00	1.097	1.179126011	1.128	1.179
					298.50	1.149	1.227848975	1.177	1.228
					310.70	1.204	1.275696566	1.225	1.276
					322.60	1.259	1.322652281	1.272	1.323
					334.30	1.308	1.369096769	1.318	1.369
					345.70	1.355	1.414618438	1.364	1.415
Tetraphenylethane	C26H20	332.44	0.138	Test set 1, Training set 2	101.90	0.466	0.474146593	0.433	0.474
					126.10	0.541	0.56638271	0.522	0.566

					147.40	0.612	0.6455856	0.600	0.646
					166.70	0.670	0.716846132	0.670	0.717
					184.40	0.731	0.782205779	0.735	0.782
					201.10	0.795	0.84408249	0.797	0.844
					216.80	0.851	0.902547224	0.855	0.903
					231.70	0.901	0.958357442	0.910	0.958
					246.00	0.951	1.01225565	0.964	1.012
					259.80	1.004	1.064605731	1.016	1.065
					273.10	1.051	1.115388692	1.067	1.115
					286.00	1.105	1.164965329	1.116	1.165
					298.50	1.164	1.213314789	1.165	1.213
					310.70	1.213	1.260804505	1.212	1.261
					322.30	1.262	1.306238691	1.257	1.306
					334.30	1.306	1.353530658	1.305	1.354
					345.70	1.349	1.398735166	1.350	1.399
1,1,2,2-Tetraphenylethane	C26H22	334.46	0.144	Test set 1, Training set 2	101.90	0.459	0.492787468	0.447	0.493
					126.10	0.534	0.587752111	0.539	0.588
					147.40	0.605	0.669109336	0.619	0.669
					166.70	0.668	0.742193354	0.691	0.742

					184.40	0.734	0.809145805	0.757	0.809
					201.10	0.799	0.872468848	0.820	0.872
					216.80	0.856	0.932250297	0.879	0.932
					231.70	0.912	0.989275602	0.936	0.989
					246.00	0.968	1.044310826	0.991	1.044
					259.80	1.028	1.097732727	1.044	1.098
					273.10	1.087	1.14952613	1.096	1.150
					286.00	1.138	1.200062455	1.146	1.200
					298.50	1.186	1.249323269	1.195	1.249
					310.70	1.231	1.297685252	1.244	1.298
					322.60	1.277	1.345132859	1.291	1.345
					334.30	1.326	1.392051632	1.338	1.392
					345.70	1.376	1.438026633	1.384	1.438
1,1,1,2-Tetraphenylethane	C26H22	334.46	0.144	Test set 1, Training set 2	101.90	0.443	0.493	0.447	0.493
					126.10	0.522	0.588	0.539	0.588
					147.40	0.588	0.669	0.619	0.669
					166.70	0.648	0.742	0.691	0.742
					184.40	0.714	0.809	0.757	0.809
					201.10	0.776	0.872	0.820	0.872

					216.80	0.842	0.932	0.879	0.932
					231.70	0.897	0.989	0.936	0.989
					246.00	0.953	1.044	0.991	1.044
					259.80	1.015	1.098	1.044	1.098
					273.10	1.073	1.150	1.096	1.150
					286.00	1.127	1.200	1.146	1.200
					298.50	1.182	1.249	1.195	1.249
					310.70	1.237	1.298	1.244	1.298
					322.60	1.289	1.345	1.291	1.345
					334.30	1.345	1.392	1.338	1.392
					345.70	1.396	1.438	1.384	1.438
11-Phenylheneicosane	C27H48	372.67	0.201	Test set 1, Training set 2	80.00	0.575	0.584	0.483	0.584
					90.00	0.625	0.642	0.535	0.642
					100.00	0.674	0.697	0.585	0.697
					110.00	0.722	0.749	0.633	0.749
					120.00	0.770	0.799	0.681	0.799
					130.00	0.814	0.848	0.727	0.848
					140.00	0.854	0.896	0.773	0.896
					150.00	0.890	0.943	0.819	0.943

					160.00	0.931	0.989	0.864	0.989
					170.00	0.970	1.035	0.909	1.035
					180.00	1.010	1.081	0.953	1.081
					190.00	1.050	1.126	0.998	1.126
					200.00	1.096	1.171	1.042	1.171
					210.00	1.145	1.216	1.087	1.216
					220.00	1.192	1.261	1.131	1.261
					230.00	1.242	1.305	1.175	1.305
					240.00	1.293	1.350	1.219	1.350
					250.00	1.343	1.394	1.263	1.394
					260.00	1.397	1.438	1.307	1.438
					270.00	1.473	1.483	1.351	1.483
p-Quinquephenyl	C30H22	382.50	0.136	Test set 1, Training set 2	50.00	0.235	0.238	0.215	0.238
					60.00	0.278	0.289	0.261	0.289
					70.00	0.314	0.335	0.303	0.335
					80.00	0.346	0.378	0.343	0.378
					90.00	0.378	0.419	0.381	0.419
					100.00	0.410	0.458	0.419	0.458
					110.00	0.445	0.496	0.456	0.496

					120.00	0.479	0.534	0.492	0.534
					130.00	0.511	0.571	0.529	0.571
					140.00	0.546	0.607	0.565	0.607
					150.00	0.582	0.644	0.601	0.644
					160.00	0.619	0.680	0.637	0.680
					170.00	0.657	0.717	0.673	0.717
					180.00	0.696	0.753	0.709	0.753
					190.00	0.735	0.790	0.745	0.790
					200.00	0.775	0.827	0.782	0.827
					210.00	0.816	0.863	0.818	0.863
					220.00	0.859	0.900	0.855	0.900
					230.00	0.903	0.937	0.892	0.937
					240.00	0.950	0.975	0.929	0.975
					250.00	0.998	1.012	0.966	1.012
Pentaphenylethane	C32H26	410.56	0.141	Test set 1, Training set 2	101.90	0.438	0.485	0.441	0.485
					126.10	0.511	0.578	0.532	0.578
					147.40	0.574	0.659	0.611	0.659
					166.70	0.634	0.731	0.682	0.731
					184.40	0.693	0.797	0.748	0.797

					201.10	0.756	0.860	0.810	0.860
					216.80	0.819	0.919	0.869	0.919
					231.70	0.875	0.976	0.925	0.976
					246.00	0.932	1.030	0.979	1.030
					259.80	0.989	1.083	1.032	1.083
					273.10	1.045	1.135	1.083	1.135
					286.00	1.099	1.185	1.133	1.185
					298.50	1.154	1.234	1.182	1.234
					310.70	1.216	1.282	1.230	1.282
					322.60	1.265	1.329	1.277	1.329
					334.30	1.305	1.375	1.324	1.375
					345.70	1.330	1.421	1.369	1.421
1,3,5-Tri-2-Naphthylbenzene	C36H24	456.59	0.131	Test set 1, Training set 2	51.15	0.229	0.235	0.214	0.235
					53.42	0.238	0.247	0.224	0.247
					55.92	0.248	0.259	0.235	0.259
					58.61	0.258	0.272	0.247	0.272
					61.42	0.268	0.285	0.259	0.285
					64.35	0.278	0.298	0.271	0.298
					67.44	0.289	0.312	0.283	0.312

					70.57	0.300	0.325	0.296	0.325
					73.59	0.310	0.338	0.308	0.338
					76.82	0.320	0.351	0.320	0.351
					80.24	0.331	0.365	0.333	0.365
					82.95	0.340	0.376	0.344	0.376
					85.34	0.347	0.386	0.353	0.386
					89.06	0.359	0.400	0.367	0.400
					93.07	0.372	0.416	0.381	0.416
					86.74	0.352	0.391	0.358	0.391
					90.48	0.364	0.406	0.372	0.406
					94.23	0.375	0.420	0.386	0.420
					98.01	0.387	0.434	0.399	0.434
					101.80	0.399	0.449	0.413	0.449
					105.62	0.411	0.463	0.427	0.463
					109.47	0.423	0.477	0.441	0.477
					113.35	0.435	0.491	0.455	0.491
					116.95	0.446	0.504	0.467	0.504
					120.45	0.457	0.517	0.480	0.517
					123.95	0.469	0.530	0.492	0.530

					127.45	0.480	0.542	0.504	0.542
					130.96	0.491	0.555	0.517	0.555
					134.37	0.502	0.567	0.529	0.567
					137.85	0.514	0.580	0.541	0.580
					141.42	0.526	0.592	0.554	0.592
					145.09	0.538	0.605	0.567	0.605
					148.86	0.551	0.619	0.580	0.619
					152.72	0.564	0.633	0.593	0.633
					156.68	0.578	0.647	0.607	0.647
					160.73	0.591	0.661	0.622	0.661
					164.87	0.606	0.676	0.636	0.676
					169.09	0.621	0.691	0.651	0.691
					173.40	0.636	0.706	0.666	0.706
					177.80	0.652	0.722	0.682	0.722
					182.29	0.668	0.738	0.698	0.738
					186.83	0.685	0.754	0.714	0.754
					191.39	0.701	0.771	0.730	0.771
					195.99	0.719	0.787	0.746	0.787
					200.63	0.736	0.804	0.763	0.804

					205.30	0.753	0.820	0.780	0.820
					210.02	0.771	0.837	0.797	0.837
					214.77	0.789	0.855	0.814	0.855
					219.55	0.808	0.872	0.831	0.872
					224.38	0.826	0.889	0.848	0.889
					229.23	0.845	0.907	0.866	0.907
					234.13	0.864	0.925	0.884	0.925
					239.06	0.884	0.943	0.902	0.943
					244.02	0.904	0.961	0.920	0.961
					249.02	0.923	0.979	0.938	0.979
					254.05	0.944	0.998	0.957	0.998
					259.22	0.964	1.017	0.976	1.017
					264.47	0.987	1.036	0.995	1.036
					269.80	1.009	1.056	1.015	1.056
					275.20	1.031	1.076	1.035	1.076
					280.66	1.053	1.097	1.055	1.097
					286.19	1.076	1.117	1.076	1.117
					291.79	1.100	1.138	1.097	1.138
					297.45	1.122	1.160	1.118	1.160

					303.18	1.145	1.181	1.140	1.181
					308.97	1.168	1.203	1.161	1.203
					314.82	1.192	1.225	1.184	1.225
					320.74	1.215	1.248	1.206	1.248
					326.72	1.239	1.271	1.229	1.271
					332.75	1.263	1.294	1.252	1.294
					338.85	1.286	1.318	1.276	1.318
					345.00	1.309	1.341	1.300	1.341
					351.21	1.332	1.366	1.324	1.366
					357.48	1.355	1.390	1.348	1.390
					363.80	1.379	1.415	1.373	1.415
					370.17	1.402	1.440	1.398	1.440

Appendix B: Liquid Isobaric Heat Capacity Database:

Compound	Formula	Molar Mass [g.mol^{-1}]	α [mol.g^{-1}]	Database	T [K]	C_{pDS} [J.K^{-1}.g^{-1}]				
						Experimental	Calculated using Dadgostar-Shaw (DS)	Calculated using the adjusted DS (chap3)	Calculated using the heteroatom corrected DS (5-1)	Calculated using the heteroatom corrected DS (5-2)
Alkanes										
Heptane	C_7H_{16}	100.2	0.230	Test set 1, Training set 2	196.42	2.003	1.774	1.819	N/A	N/A
					208.55	2.007	1.820	1.865		
					220.61	2.011	1.865	1.911		
					229.57	2.037	1.899	1.945		
					238.45	2.057	1.933	1.978		
					250.18	2.087	1.977	2.022		
					261.78	2.117	2.020	2.066		
					270.39	2.147	2.053	2.098		
					276.20	2.166	2.074	2.120		
					281.74	2.185	2.095	2.140		
					287.37	2.199	2.116	2.161		
					295.68	2.228	2.147	2.192		

					308.45	2.278	2.194	2.239		
					317.91	2.318	2.229	2.274		
					330.38	2.368	2.275	2.320		
					336.54	2.394	2.297	2.343		
					342.66	2.421	2.320	2.365		
2,2,3,3-Tetramethylpentane	C_9H_{20}	128.26	0.226	Training set 1, Training set 2	223.20	1.986	2.032	2.079		
					227.50	2.015	2.056	2.103		
					244.50	2.036	2.074	2.121		
					275.00	2.099	2.126	2.172		
					278.20	2.132	2.155	2.201		
					283.30	2.219	2.225	2.272		
					289.40	2.305	2.296	2.343		
					295.00	2.365	2.342	2.389		
2,7-Dimethyloctane, Diisoamyl	$C_{10}H_{22}$	142.28	0.225	Training set 1,Training set 2	223.20	1.895	1.848	1.895		
					227.50	1.904	1.865	1.912		
					244.50	1.954	1.931	1.978		
					275.00	2.059	2.048	2.096		
					278.20	2.063	2.060	2.108		
					283.30	2.084	2.080	2.127		

					289.40	2.096	2.103	2.150		
					295.00	2.121	2.124	1.895		
Decane	$C_{10}H_{22}$	142.28	0.225	Test set 1, Training set 2	318.15	2.276	2.211	2.259		
					333.15	2.333	2.267	2.314		
					348.15	2.393	2.322	2.370		
					363.15	2.456	2.377	2.425		
					373.15	2.504	2.414	2.259		
2-Methyldecane	$C_{11}H_{24}$	156.31	0.224	Training set 1, Training set 2	235.44	2.001	1.890	1.938		
					240.66	2.012	1.911	1.958		
					248.28	2.027	1.940	1.988		
					257.24	2.050	1.975	2.023		
					276.59	2.109	2.050	2.097		
					295.78	2.174	2.123	2.171		
					311.95	2.236	2.184	2.232		
					332.25	2.315	2.260	2.307		
					342.46	2.357	2.298	2.345		
					356.08	2.410	2.348	2.396		
					375.23	2.494	2.418	2.465		
					280.15	2.166	2.056	2.104		

Tridecane	$C_{13}H_{28}$	184.36	0.222	Training set 1, Training set 2	288.15	2.182	2.087	2.135		
					298.15	2.207	2.125	2.173		
					308.15	2.235	2.163	2.211		
					318.15	2.265	2.201	2.249		
Pentadecane	$C_{15}H_{32}$	212.42	0.221	Test set 1, Training set 2	313.15	2.250	2.177	2.226		
					333.15	2.313	2.252	2.301		
					353.15	2.378	2.326	2.375		
					373.15	2.444	2.400	2.448		
Hexadecane	$C_{16}H_{34}$	226.45	0.221	Training set 1, Training set 2	318.15	2.263	2.194	2.243		
					328.15	2.278	2.231	2.280		
					338.15	2.320	2.269	2.318		
					348.15	2.351	2.306	2.355		
					358.15	2.385	2.343	2.392		
					368.15	2.421	2.379	2.428		
Octadecane	$C_{18}H_{38}$	254.49	0.220	Test set 1, Training set 2	306.69	2.247	2.147	2.196		
					314.63	2.266	2.177	2.227		
					322.51	2.289	2.207	2.256		
					330.34	2.312	2.236	2.286		
					338.13	2.336	2.266	2.315		

					345.90	2.361	2.295	2.344		
					353.61	2.388	2.323	2.372		
					361.27	2.415	2.351	2.401		
					368.87	2.443	2.379	2.428		
					376.43	2.468	2.407	2.456		
					383.66	2.499	2.433	2.482		
					391.14	2.527	2.460	2.509		
					398.59	2.553	2.486	2.536		
Naphtenes										
Butylcyclohexane	$C_{10}H_{20}$	140.27	0.214	Training set 1, Training set 2	207.52	1.622	1.715	1.604	N/A	N/A
					214.21	1.640	1.743	1.632		
					221.77	1.660	1.775	1.664		
					240.10	1.717	1.851	1.741		
					260.05	1.785	1.933	1.822		
					280.56	1.861	2.016	1.905		
					290.54	1.901	2.055	1.944		
					305.97	1.965	2.116	2.005		
					325.86	2.049	2.192	2.081		
					345.43	2.132	2.266	2.155		

					365.38	2.219	2.340	2.229		
Decylcyclopentane	$C_{15}H_{30}$	210.40	0.214	Test set 1, Training set 2	258.18	1.930	1.926	1.815		
					264.82	1.939	1.952	1.842		
					271.95	1.953	1.981	1.870		
					282.67	1.980	2.024	1.913		
					299.44	2.030	2.090	1.979		
					311.43	2.071	2.137	2.026		
Decylcyclohexane	$C_{16}H_{32}$	224.34	0.214	Training set 1, Training set 2	274.26	1.940	1.991	1.880		
					280.27	1.958	2.015	1.904		
					286.10	1.976	2.038	1.927		
					293.33	2.000	2.067	1.956		
					300.48	2.024	2.095	1.984		
1,1,3-Tricyclohexylpropane	$C_{21}H_{38}$	290.53	0.203	Training set 1, Training set 2	373.15	2.198	2.316	2.223		
					423.15	2.415	2.490	2.397		
					483.15	2.633	2.681	2.588		
Aromatics & Unsaturated Cyclic Hydrocarbons										
Styrene	C_8H_8	104.15	0.154	Test set 1, Training set 2	246.73	1.614	1.484	1.424	N/A	N/A
					249.91	1.625	1.499	1.439		
					257.54	1.630	1.534	1.473		

					276.24	1.686	1.616	1.556		
					298.54	1.753	1.710	1.650		
Dimethylbenzene	C_8H_{10}	106.17	0.170	Training set 1, Training set 2	251.99	1.642	1.623	1.617		
					255.57	1.651	1.639	1.633		
					262.25	1.668	1.669	1.664		
					285.47	1.731	1.771	1.765		
					297.74	1.767	1.822	1.817		
Naphthalene	$C_{10}H_8$	128.17	0.140	Training set 1, Training set 2	357.43	1.709	1.821	1.717		
					358.66	1.713	1.825	1.721		
					362.48	1.724	1.838	1.734		
					374.96	1.762	1.878	1.774		
					401.99	1.845	1.959	1.855		
					427.29	1.921	2.027	1.923		
1-Methylnaphthalene	$C_{11}H_{10}$	142.2	0.148	Test set 1, Training set 2	247.97	1.439	1.446	1.361		
					257.51	1.463	1.489	1.404		
					266.59	1.487	1.529	1.444		
					286.39	1.543	1.614	1.529		
					299.90	1.583	1.670	1.585		
					310.24	1.615	1.711	1.626		

					330.80	1.678	1.789	1.704		
					352.19	1.744	1.866	1.781		
Anthracene	$C_{14}H_{10}$	178.23	0.135	Training set 1, Training set 2	495.00	2.249	2.112	1.994		
					497.00	2.377	2.116	1.997		
					498.15	2.355	2.117	1.999		
					500.00	2.425	2.121	2.002		
					502.00	2.409	2.124	2.005		
trans-Stilbene	$C_{14}H_{12}$	180.24	0.144	Test set 1, Training set 2	401.61	1.962	1.993	1.898		
					404.6	1.968	2.002	1.907		
					407.59	1.976	2.010	1.915		
					410.57	1.984	2.019	1.924		
Pyrene	$C_{16}H_{10}$	202.25	0.129	Training set 1, Training set 2	430.70	1.742	1.915	1.783		
					440.32	1.771	1.937	1.805		
					449.86	1.798	1.958	1.826		
					459.30	1.823	1.978	1.845		
					468.98	1.849	1.997	1.864		
					478.79	1.878	2.015	1.883		
o-Terphenyl	$C_{18}H_{14}$	230.31	0.139	Training set 1,	330.10	1.693	1.713	1.605		
					336.85	1.712	1.737	1.629		

				Training set 2	355.60	1.765	1.802	1.694		
Benzo[a]pyrene	$C_{20}H_{12}$	252.3	0.127	Training set 1, Training set 2	457.23	1.829	1.955	1.817		
					466.64	1.844	1.973	1.835		
					476.56	1.873	1.992	1.854		
					486.48	1.887	2.009	1.871		
					496.40	1.915	2.025	1.887		
Compounds with heteroatoms (SNO)										
2-Aminobiphenyl	C12H11N	169.23	0.142	Training set 1, Training set 2	295.39	1.755	1.604	1.668	N/A	N/A
					311.51	1.792	1.668	1.731		
					328.48	1.832	1.732	1.795		
					329.26	1.834	1.735	1.798		
					332.33	1.841	1.746	1.809		
					338.26	1.855	1.767	1.831		
					358.18	1.904	1.836	1.900		
					387.10	1.975	1.928	1.992		
					415.74	2.046	2.010	2.074		
					440.49	2.107	2.074	2.138		
					327.75	1.514	1.611	1.672		
					331.19	1.524	1.623	1.684		

Benzo[h]quinoline	C13H9N	179.22	0.128	Training set 1, Training set 2	337.10	1.540	1.643	1.704		
					346.81	1.568	1.676	1.737		
					369.21	1.632	1.747	1.808		
					393.49	1.701	1.818	1.879		
					405.62	1.735	1.850	1.912		
					428.34	1.797	1.907	1.969		
Diphenyl Methanone	C13H10O	182.21	0.132	Test set 1, Training set 2	271.42	1.518	1.422	1.463	1.461	1.465
					277.98	1.533	1.450	1.491	1.489	1.493
					288.10	1.558	1.491	1.532	1.530	1.535
					301.81	1.592	1.545	1.586	1.584	1.589
					316.88	1.632	1.602	1.643	1.641	1.647
					331.75	1.671	1.655	1.697	1.695	1.701
					344.93	1.707	1.701	1.742	1.740	1.747
					358.40	1.743	1.745	1.786	1.784	1.792
					373.57	1.784	1.793	1.834	1.832	1.840
					388.99	1.825	1.838	1.880	1.878	1.887
					404.59	1.867	1.882	1.923	1.921	1.931
					429.95	1.933	1.947	1.988	1.986	1.996
1,2,3,4-	C12H12S	188.29	0.133	Test set 1,	287.64	1.396	1.498	1.540	N/A	N/A

Tetrahydrodibenzothiophene				Training set 2	300.54	1.430	1.549	1.591		
					315.41	1.471	1.606	1.648		
					330.79	1.515	1.662	1.704		
9-Fluorenemethanol	C14H12O	196.24	0.138	Training set 1, Training set 2	378.40	2.127	1.863	1.930	1.903	1.911
					381.41	2.193	1.872	1.939	1.912	1.920
					385.71	2.276	1.885	1.952	1.925	1.933
					389.69	2.346	1.897	1.964	1.937	1.945
1,1' -Thiobis(cyclohexane)	C12H22S	198.37	0.176	Training set 1, Training set 2	287.60	1.610	1.826	1.892	N/A	N/A
					290.60	1.620	1.839	1.904		
					307.92	1.676	1.911	1.976		
					336.79	1.777	2.024	2.089		
					367.76	1.890	2.138	2.203		
					398.09	2.005	2.241	2.307		
					428.06	2.120	2.336	2.402		
Carboxine	C12H13NO2S	235.302	0.123	Training set 1, Training set 2	367.32	1.844	1.691	1.751	1.752	1.764
					370.32	1.865	1.700	1.760	1.761	1.773
					374.78	1.881	1.713	1.774	1.774	1.787
					377.65	1.899	1.722	1.782	1.782	1.795
					380.54	1.913	1.730	1.790	1.790	1.804

N-Octyl-1-octanamine	C16H35N	241.46	0.215	Test set 1, Training set 2	300.00	2.107	2.099	1.751	N/A	N/A
					340.00	2.283	2.252	1.760		
					380.00	2.441	2.399	1.774		
					420.00	2.586	2.541	1.782		
					460.00	2.720	2.677	1.790		
					500.00	2.848	2.807	1.751		
					540.00	2.979	2.932	1.760		
					580.00	3.113	3.051	1.774		
Ethyl Tridecanoate	C15H30O	242.398	0.194	Training set 1, Training set 2	275.34	2.006	1.884	1.948	1.942	1.949
					278.01	2.010	1.895	1.959	1.954	1.960
					280.68	2.016	1.906	1.970	1.965	1.972
					283.33	2.018	1.917	1.981	1.976	1.983
					285.99	2.019	1.928	1.992	1.987	1.994
					288.64	2.024	1.939	2.003	1.998	2.005
					291.29	2.030	1.950	2.014	2.009	2.017
					293.93	2.034	1.961	2.025	2.020	2.028
					296.56	2.041	1.972	2.036	2.031	2.039
					299.20	2.046	1.983	2.047	2.042	2.050
					301.82	2.052	1.993	2.058	2.052	2.060

					304.44	2.058	2.004	2.068	2.063	2.071
					307.06	2.066	2.015	2.079	2.073	2.082
					309.67	2.073	2.025	2.089	2.084	2.093
Molten polymers:										
Isotactic Polypropylene	(C3H6)n	42.08	0.214	Training set 1, Training set 2	450.00	2.719	2.636	2.638	N/A	N/A
					470.00	2.777	2.702	2.704		
					490.00	2.834	2.767	2.769		
					510.00	2.885	2.830	2.832		
					530.00	2.932	2.892	2.894		
					550.00	2.973	2.952	2.954		
					570.00	3.012	3.010	3.013		
					590.00	3.048	3.068	3.070		
Poly(1-butene)	(C4H8)n	56.11	0.214	Test set 1, Training set 2	420.00	2.491	2.534	2.533		
					440.00	2.550	2.602	2.601		
					460.00	2.610	2.669	2.668		
					480.00	2.670	2.735	2.733		
					500.00	2.729	2.799	2.797		
					520.00	2.789	2.861	2.860		
					540.00	2.856	2.922	2.920		

					560.00	2.927	2.981	2.980		
					580.00	2.998	3.039	3.038		
					600.00	3.076	3.095	3.094		
					620.00	3.158	3.150	3.149		
Atatic Poly(methyl methacrylate)	(C5O2H8)n	100.12	0.150	Test set 1, Training set 2	430.00	2.131	2.123	2.085		
					450.00	2.181	2.174	2.136		
					470.00	2.232	2.221	2.182		
					490.00	2.282	2.263	2.225		
					510.00	2.328	2.302	2.263		
					530.00	2.378	2.336	2.297		
					550.00	2.424	2.365	2.327		
Polystyrene	(C8H8)n	104.15	0.154	Training set 1, Training set 2	420.00	2.017	2.129	2.094		
					440.00	2.077	2.184	2.149		
					460.00	2.137	2.234	2.199		
					480.00	2.193	2.280	2.245		
					500.00	2.246	2.321	2.287		
					520.00	2.294	2.359	2.324		
					540.00	2.342	2.392	2.358		
					560.00	2.386	2.421	2.387		

					580.00	2.430	2.446	2.412		
Poly (oxy-2,6-dimethyl-1,4-phenylene)	(C6H2(CH3)2O)n	120.15	0.141	Training set 1, Training set 2	534.44	2.194	2.250	2.212		
					544.17	2.213	2.263	2.225		
Poly (oxyoctamethylene)	((CH2)8O)n	128.21	0.195	Test set 1, Training set 2	347.61	2.268	2.180	2.165		
					350.43	2.209	2.191	2.175		
					353.47	2.224	2.202	2.187		

Appendix C: MATLAB script (Liquid Paraffin Example)

```
clc

a_11=-0.341624453510121;
a_12=2.26706901789294;
b_11=0.106424258819175;
b_12=-0.387375462437376;
c_11=-0.000098231239195945;
c_12=0.000418199793943863;
x=[a_11,a_12,b_11,b_12,c_11,c_12];
X=[24.5.*Alpha_P, 24.5.*(Alpha_P.^2),...
   Alpha_P.*T_P,(Alpha_P.^2).*T_P,...
   Alpha_P.*(T_P.^2),(Alpha_P.^2).*(T_P.^2)];

n=-1:0.01:1;
k=1;
```

```
for i=1:length(n)

   a11(i)=a_11+ a_11*n(i);
 for j=1:length(n)
   a12(j)=a_12+a_12*n(j);
   %x=[a11(i),a12(j),b_11,b_12,c_11,c_12];
   Cp_P(1:38,k)= 24.5.*Alpha_P.*a11(i)+ 24.5.*(Alpha_P.^2).*a12(j)...
   +Alpha_P.*T_P.*b_11+(Alpha_P.^2).*T_P.*b_12...
   +Alpha_P.*(T_P.^2).*c_11+(Alpha_P.^2).*(T_P.^2).*c_12;

   Err_r(k)= mean(abs(Cp_P(1:38,k)-Cpexp_P)./Cpexp_P);

   k=k+1;
   index=[k;i;j]
 end
end
[er,in]=min(Err_r)
```

Appendix D: Solid Isobaric Heat Capacity Database of Sugars and their Melting Points

Name	Formula	M [g.mol^{-1}]	α [mol.g^{-1}]	Database	T [K]	C_{pLS} [J.K^{-1}.g^{-1}]		
						Experimental	Calculated using Lastovka-Shaw (LS)	Calculated using the heteroatom corrected LS (chap4)
Glucose	C6H12O6	180.2	0.133	Test set 2	352.7	1.452	1.385	1.554
					352.9	1.453	1.386	1.555
					353.1	1.454	1.386	1.556
					353.2	1.455	1.387	1.556
					353.4	1.455	1.388	1.557
					353.6	1.456	1.388	1.557
					353.7	1.455	1.389	1.558
					353.9	1.458	1.390	1.559
					354.1	1.460	1.390	1.559
					354.2	1.459	1.391	1.560
					354.4	1.461	1.391	1.561

					354.6	1.460	1.392	1.561
					354.7	1.461	1.393	1.562
					354.9	1.462	1.393	1.563
					355.1	1.462	1.394	1.563
					355.2	1.463	1.395	1.564
					355.4	1.464	1.395	1.565
					355.6	1.464	1.396	1.565
					355.7	1.464	1.397	1.566
					355.9	1.466	1.397	1.567
					356.1	1.466	1.398	1.567
					356.2	1.467	1.399	1.568
					356.4	1.468	1.399	1.569
					356.6	1.468	1.400	1.569
					356.7	1.470	1.401	1.570
					356.9	1.470	1.401	1.571
					357.1	1.471	1.402	1.571
Glucose	C6H12O6	180.2	0.133	Test set 2	357.2	1.471	1.403	1.572
					357.4	1.473	1.403	1.573

					357.6	1.472	1.404	1.573
					357.7	1.474	1.405	1.574
					357.9	1.474	1.405	1.575
					358.1	1.475	1.406	1.575
					358.2	1.476	1.407	1.576
					358.4	1.475	1.407	1.577
					358.6	1.477	1.408	1.577
					358.7	1.477	1.409	1.578
					358.9	1.479	1.409	1.578
					359.1	1.478	1.410	1.579
					359.3	1.480	1.411	1.580
					359.4	1.480	1.411	1.580
					359.6	1.481	1.412	1.581
					359.8	1.481	1.412	1.582
					359.9	1.483	1.413	1.582
					360.1	1.484	1.414	1.583
					360.2	1.485	1.414	1.584
					360.4	1.484	1.415	1.584

					360.6	1.485	1.416	1.585
					360.7	1.485	1.416	1.586
					360.9	1.486	1.417	1.586
					361.1	1.486	1.418	1.587
					361.2	1.487	1.418	1.588
					361.4	1.488	1.419	1.588
					361.6	1.488	1.420	1.589
					361.7	1.489	1.420	1.590
					361.9	1.490	1.421	1.590
					362.1	1.490	1.422	1.591
					362.3	1.491	1.422	1.592
					362.4	1.492	1.423	1.592
					362.6	1.493	1.424	1.593
					362.8	1.493	1.424	1.594
					362.9	1.494	1.425	1.594
Glucose	C6H12O6	180.2	0.133	Test set 2	363.1	1.494	1.426	1.595
					363.3	1.496	1.426	1.596
					363.4	1.496	1.427	1.596

					363.6	1.497	1.428	1.597
					363.8	1.498	1.428	1.597
					363.9	1.500	1.429	1.598
					364.1	1.499	1.430	1.599
					364.3	1.499	1.430	1.599
					364.4	1.501	1.431	1.600
					364.6	1.502	1.432	1.601
					364.8	1.503	1.432	1.601
					364.9	1.504	1.433	1.602
					365.1	1.503	1.433	1.603
					365.3	1.504	1.434	1.603
					365.4	1.506	1.435	1.604
					365.6	1.506	1.435	1.605
					365.8	1.507	1.436	1.605
					365.9	1.507	1.437	1.606
					366.1	1.508	1.437	1.607
					366.3	1.509	1.438	1.607
					366.4	1.509	1.439	1.608

					366.6	1.510	1.439	1.609
					366.8	1.512	1.440	1.609
					366.9	1.512	1.441	1.610
					367.1	1.514	1.441	1.611
					367.3	1.515	1.442	1.611
					367.4	1.516	1.443	1.612
					367.6	1.516	1.443	1.613
					367.8	1.517	1.444	1.613
					367.9	1.519	1.445	1.614
					368.1	1.519	1.445	1.615
					368.3	1.519	1.446	1.615
					368.4	1.520	1.447	1.616
					368.6	1.521	1.447	1.617
					368.8	1.521	1.448	1.617
Glucose	C6H12O6	180.2	0.133	Test set 2	368.9	1.522	1.449	1.618
					369.1	1.523	1.449	1.619
					369.3	1.524	1.450	1.619
					369.4	1.524	1.451	1.620

					369.6	1.526	1.451	1.621
					369.8	1.527	1.452	1.621
					369.9	1.528	1.453	1.622
					370.1	1.528	1.453	1.622
					370.3	1.530	1.454	1.623
					370.4	1.531	1.455	1.624
					370.6	1.530	1.455	1.624
					370.8	1.532	1.456	1.625
					370.9	1.533	1.457	1.626
					371.1	1.534	1.457	1.626
					371.3	1.534	1.458	1.627
					371.4	1.534	1.458	1.628
					371.6	1.536	1.459	1.628
					371.8	1.536	1.460	1.629
					371.9	1.538	1.460	1.630
					372.1	1.538	1.461	1.630
					372.3	1.540	1.462	1.631
					372.4	1.539	1.462	1.632

					372.6	1.541	1.463	1.632
					372.8	1.542	1.464	1.633
					372.9	1.543	1.464	1.634
					373.1	1.543	1.465	1.634
					373.3	1.544	1.466	1.635
					373.4	1.545	1.466	1.636
					373.6	1.545	1.467	1.636
					373.8	1.547	1.468	1.637
					373.9	1.548	1.468	1.638
					374.1	1.548	1.469	1.638
					374.3	1.550	1.470	1.639
					374.4	1.550	1.470	1.640
					374.6	1.551	1.471	1.640
Glucose	C6H12O6	180.2	0.133	Test set 2	374.8	1.552	1.472	1.641
					374.9	1.553	1.472	1.642
					375.1	1.554	1.473	1.642
					375.3	1.554	1.474	1.643
					375.4	1.556	1.474	1.644

					375.6	1.556	1.475	1.644
					375.8	1.558	1.476	1.645
					375.9	1.558	1.476	1.646
					376.1	1.558	1.477	1.646
					376.3	1.559	1.478	1.647
					376.4	1.561	1.478	1.648
					376.6	1.561	1.479	1.648
					376.8	1.562	1.480	1.649
					376.9	1.562	1.480	1.650
					377.1	1.563	1.481	1.650
					377.3	1.563	1.482	1.651
					377.4	1.564	1.482	1.652
					377.6	1.565	1.483	1.652
					377.8	1.566	1.484	1.653
					377.9	1.566	1.484	1.654
					378.1	1.567	1.485	1.654
					378.3	1.568	1.486	1.655
					378.4	1.570	1.486	1.656

					378.6	1.571	1.487	1.656
					378.8	1.571	1.488	1.657
					378.9	1.571	1.488	1.657
					379.1	1.572	1.489	1.658
					379.3	1.573	1.490	1.659
					379.4	1.573	1.490	1.659
					379.6	1.574	1.491	1.660
					379.8	1.576	1.492	1.661
					379.9	1.576	1.492	1.661
					380.1	1.578	1.493	1.662
					380.3	1.579	1.494	1.663
					380.4	1.580	1.494	1.663
	C6H12O6	180.2	0.133	Test set 2	380.6	1.579	1.495	1.664
					380.8	1.581	1.495	1.665
					380.9	1.582	1.496	1.665
					381.1	1.582	1.497	1.666
					381.3	1.584	1.497	1.667
					381.4	1.584	1.498	1.667

					381.6	1.585	1.499	1.668
					381.8	1.585	1.499	1.669
					381.9	1.586	1.500	1.669
					382.1	1.587	1.501	1.670
					382.3	1.588	1.501	1.671
					382.4	1.589	1.502	1.671
					382.6	1.590	1.503	1.672
					382.8	1.591	1.503	1.673
					382.9	1.591	1.504	1.673
					383.1	1.592	1.505	1.674
					383.3	1.593	1.505	1.675
					383.4	1.594	1.506	1.675
					383.6	1.595	1.507	1.676
					383.8	1.596	1.507	1.677
					383.9	1.596	1.508	1.677
					384.1	1.597	1.509	1.678
					384.2	1.599	1.509	1.679
					384.4	1.600	1.510	1.679

					384.6	1.601	1.511	1.680
					384.7	1.601	1.511	1.681
					384.9	1.602	1.512	1.681
					385.1	1.602	1.513	1.682
					385.2	1.603	1.513	1.683
					385.4	1.605	1.514	1.683
					385.6	1.605	1.515	1.684
					385.7	1.607	1.515	1.685
					385.9	1.607	1.516	1.685
					386.1	1.608	1.517	1.686
					386.2	1.608	1.517	1.687
Glucose	C6H12O6	180.2	0.133	Test set 2	386.4	1.610	1.518	1.687
					386.6	1.610	1.519	1.688
					386.7	1.611	1.519	1.689
					386.9	1.611	1.520	1.689
					387.1	1.613	1.521	1.690
					387.2	1.613	1.521	1.691
					387.4	1.615	1.522	1.691

					387.6	1.616	1.523	1.692
					387.7	1.617	1.523	1.693
					387.9	1.617	1.524	1.693
					388.1	1.618	1.525	1.694
					388.2	1.618	1.525	1.695
					388.4	1.620	1.526	1.695
					388.6	1.621	1.527	1.696
					388.7	1.622	1.527	1.697
					388.9	1.623	1.528	1.697
					389.1	1.623	1.529	1.698
					389.2	1.624	1.529	1.699
					389.4	1.625	1.530	1.699
					389.6	1.625	1.531	1.700
					389.7	1.626	1.531	1.701
					389.9	1.627	1.532	1.701
					390.1	1.627	1.533	1.702
					390.2	1.628	1.533	1.703
					390.4	1.630	1.534	1.703

					390.6	1.630	1.535	1.704
					390.7	1.631	1.535	1.705
					390.9	1.632	1.536	1.705
					391.1	1.633	1.537	1.706
					391.2	1.632	1.537	1.707
					391.4	1.635	1.538	1.707
					391.6	1.634	1.539	1.708
					391.7	1.636	1.539	1.709
					391.9	1.637	1.540	1.709
					392.1	1.637	1.541	1.710
Glucose	C6H12O6	180.2	0.133	Test set 2	392.2	1.639	1.541	1.711
					392.4	1.639	1.542	1.711
					392.6	1.640	1.543	1.712
					392.7	1.641	1.543	1.713
					392.9	1.641	1.544	1.713
					393.1	1.643	1.545	1.714
					393.2	1.644	1.545	1.715
					393.4	1.645	1.546	1.715

					393.6	1.646	1.547	1.716
					393.7	1.646	1.547	1.717
					393.9	1.647	1.548	1.717
					394.1	1.648	1.549	1.718
					394.2	1.649	1.549	1.719
					394.4	1.650	1.550	1.719
					394.6	1.651	1.551	1.720
					394.7	1.650	1.551	1.721
					394.9	1.652	1.552	1.721
					395.1	1.652	1.553	1.722
					395.2	1.653	1.553	1.723
					395.4	1.655	1.554	1.723
					395.6	1.656	1.555	1.724
					395.7	1.656	1.555	1.725
					395.9	1.657	1.556	1.725
					396.1	1.658	1.557	1.726
					396.2	1.660	1.557	1.727
					396.4	1.660	1.558	1.727

					396.6	1.662	1.559	1.728
					396.7	1.661	1.559	1.729
					396.9	1.663	1.560	1.729
					397.1	1.665	1.561	1.730
					397.2	1.665	1.561	1.731
					397.4	1.667	1.562	1.731
					397.6	1.668	1.563	1.732
					397.7	1.669	1.563	1.733
					397.9	1.669	1.564	1.733
Glucose	C6H12O6	180.2	0.133	Test set 2	398.1	1.670	1.565	1.734
					398.2	1.671	1.565	1.735
					398.4	1.672	1.566	1.735
					398.6	1.673	1.567	1.736
					398.7	1.674	1.567	1.737
					398.9	1.675	1.568	1.737
					399.1	1.677	1.569	1.738
					399.2	1.677	1.569	1.739
					399.4	1.678	1.570	1.739

					399.6	1.679	1.571	1.740
					399.7	1.679	1.571	1.741
					399.9	1.682	1.572	1.741
					400.1	1.683	1.573	1.742
					400.2	1.683	1.573	1.743
					400.4	1.685	1.574	1.743
					400.6	1.686	1.575	1.744
					400.7	1.687	1.575	1.745
					400.9	1.687	1.576	1.745
					401.1	1.688	1.577	1.746
					401.2	1.689	1.577	1.747
					401.4	1.691	1.578	1.747
					401.5	1.691	1.579	1.748
					401.7	1.693	1.579	1.749
					401.9	1.694	1.580	1.749
					402.1	1.695	1.581	1.750
					402.2	1.697	1.581	1.751
					402.4	1.697	1.582	1.751

					402.5	1.697	1.583	1.752
					402.7	1.698	1.583	1.753
					402.9	1.700	1.584	1.753
					403.0	1.700	1.585	1.754
					403.2	1.701	1.585	1.755
					403.4	1.703	1.586	1.755
					403.5	1.703	1.587	1.756
					403.7	1.705	1.587	1.757
Glucose	C6H12O6	180.2	0.133	Test set 2	403.9	1.706	1.588	1.757
					404.0	1.706	1.589	1.758
					404.2	1.707	1.589	1.759
					404.4	1.708	1.590	1.759
					404.5	1.708	1.591	1.760
					404.7	1.709	1.591	1.761
					404.9	1.710	1.592	1.761
					405.0	1.712	1.593	1.762
					405.2	1.713	1.593	1.763
					405.4	1.713	1.594	1.763

					405.5	1.715	1.595	1.764
					405.7	1.715	1.595	1.765
					405.9	1.715	1.596	1.765
					406.0	1.716	1.597	1.766
					406.2	1.717	1.597	1.767
					406.4	1.719	1.598	1.767
					406.5	1.720	1.599	1.768
					406.7	1.722	1.599	1.769
					406.9	1.724	1.600	1.769
					407.0	1.724	1.601	1.770
					407.2	1.725	1.601	1.771
					407.4	1.725	1.602	1.771
					407.5	1.727	1.603	1.772
					407.7	1.728	1.603	1.773
					407.9	1.730	1.604	1.773
					408.0	1.732	1.605	1.774
					408.2	1.732	1.605	1.775
					408.4	1.732	1.606	1.775

					408.5	1.735	1.607	1.776
					408.7	1.735	1.607	1.777
					408.9	1.736	1.608	1.777
					409.0	1.738	1.609	1.778
					409.2	1.738	1.609	1.779
					409.4	1.739	1.610	1.779
					409.5	1.740	1.611	1.780
Glucose	C6H12O6	180.2	0.133	Test set 2	409.7	1.743	1.611	1.781
					409.9	1.743	1.612	1.781
					410.0	1.744	1.613	1.782
					410.2	1.746	1.613	1.783
					410.4	1.748	1.614	1.783
					410.5	1.750	1.615	1.784
					410.7	1.752	1.615	1.785
					410.9	1.753	1.616	1.785
					411.0	1.754	1.617	1.786
					411.2	1.756	1.617	1.787
					411.4	1.758	1.618	1.787

					411.5	1.759	1.619	1.788
					411.7	1.761	1.619	1.789
					411.9	1.762	1.620	1.789
					412.0	1.764	1.621	1.790
					412.2	1.765	1.622	1.791
					412.4	1.768	1.622	1.791
					412.5	1.769	1.623	1.792
					412.7	1.772	1.624	1.793
					412.8	1.774	1.624	1.794
					413.0	1.776	1.625	1.794
					413.2	1.777	1.626	1.795
					413.3	1.779	1.626	1.796
					413.5	1.781	1.627	1.796
					413.7	1.784	1.628	1.797
					413.8	1.786	1.628	1.798
					414.0	1.789	1.629	1.798
					414.2	1.791	1.630	1.799
					414.3	1.794	1.630	1.800

					414.5	1.796	1.631	1.800
					414.7	1.800	1.632	1.801
					414.8	1.803	1.632	1.802
					415.0	1.805	1.633	1.802
					415.2	1.808	1.634	1.803
Maltose	C12H22O11	342.3	0.135	Test set 2	335.0	1.368	1.316	1.485
					335.2	1.368	1.317	1.486
					335.3	1.369	1.317	1.486
					335.5	1.370	1.318	1.487
					335.6	1.370	1.318	1.488
					335.8	1.371	1.319	1.488
					335.9	1.371	1.319	1.489
					336.1	1.372	1.320	1.489
					336.2	1.372	1.321	1.490
					336.4	1.372	1.321	1.491
					336.5	1.372	1.322	1.491
					336.7	1.372	1.322	1.492
					336.8	1.371	1.323	1.492

					337.0	1.370	1.324	1.493
					337.2	1.370	1.324	1.494
					337.3	1.369	1.325	1.494
					337.5	1.369	1.325	1.495
					337.6	1.368	1.326	1.495
					337.8	1.368	1.327	1.496
					337.9	1.367	1.327	1.496
					338.1	1.367	1.328	1.497
					338.2	1.366	1.328	1.498
					338.4	1.366	1.329	1.498
					338.5	1.368	1.330	1.499
					338.7	1.368	1.330	1.499
					338.8	1.369	1.331	1.500
					339.0	1.370	1.331	1.501
					339.1	1.370	1.332	1.501
					339.3	1.370	1.332	1.502
					339.4	1.372	1.333	1.502
					339.6	1.374	1.334	1.503

					339.7	1.377	1.334	1.504
					339.9	1.378	1.335	1.504
					340.0	1.379	1.335	1.505
					340.2	1.381	1.336	1.505
					340.3	1.380	1.337	1.506
Maltose	C12H22O11	342.3	0.135	Test set 2	340.5	1.381	1.337	1.506
					340.6	1.383	1.338	1.507
					340.8	1.382	1.338	1.508
					340.9	1.382	1.339	1.508
					341.1	1.382	1.340	1.509
					341.3	1.381	1.340	1.509
					341.4	1.381	1.341	1.510
					341.6	1.382	1.341	1.511
					341.7	1.384	1.342	1.511
					341.9	1.384	1.342	1.512
					342.0	1.385	1.343	1.512
					342.2	1.385	1.344	1.513
					342.3	1.385	1.344	1.514

					342.5	1.384	1.345	1.514
					342.6	1.385	1.345	1.515
					342.8	1.386	1.346	1.515
					342.9	1.388	1.347	1.516
					343.1	1.389	1.347	1.516
					343.2	1.390	1.348	1.517
					343.4	1.391	1.348	1.518
					343.5	1.391	1.349	1.518
					343.7	1.394	1.350	1.519
					343.8	1.396	1.350	1.519
					344.0	1.396	1.351	1.520
					344.1	1.397	1.351	1.521
					344.3	1.397	1.352	1.521
					344.4	1.397	1.353	1.522
					344.6	1.397	1.353	1.522
					344.7	1.397	1.354	1.523
					344.9	1.397	1.354	1.524
					345.0	1.397	1.355	1.524

					345.2	1.396	1.355	1.525
					345.3	1.396	1.356	1.525
					345.5	1.397	1.357	1.526
					345.6	1.398	1.357	1.527
Maltose	C12H22O11	342.3	0.135	Test set 2	345.8	1.398	1.358	1.527
					345.9	1.398	1.358	1.528
					346.1	1.400	1.359	1.528
					346.2	1.400	1.360	1.529
					346.4	1.400	1.360	1.529
					346.5	1.401	1.361	1.530
					346.7	1.402	1.361	1.531
					346.9	1.402	1.362	1.531
					347.0	1.403	1.363	1.532
					347.2	1.404	1.363	1.532
					347.3	1.406	1.364	1.533
					347.5	1.407	1.364	1.534
					347.6	1.407	1.365	1.534
					347.8	1.407	1.365	1.535

					347.9	1.408	1.366	1.535
					348.1	1.409	1.367	1.536
					348.2	1.410	1.367	1.537
					348.4	1.410	1.368	1.537
					348.5	1.411	1.368	1.538
					348.7	1.412	1.369	1.538
					348.8	1.412	1.370	1.539
					349.0	1.414	1.370	1.539
					349.1	1.414	1.371	1.540
					349.3	1.416	1.371	1.541
					349.4	1.417	1.372	1.541
					349.6	1.419	1.373	1.542
					349.7	1.420	1.373	1.542
					349.9	1.422	1.374	1.543
					350.0	1.423	1.374	1.544
					350.2	1.424	1.375	1.544
					350.3	1.425	1.376	1.545
					350.5	1.425	1.376	1.545

					350.6	1.427	1.377	1.546
					350.8	1.427	1.377	1.547
					350.9	1.427	1.378	1.547
Maltose	C12H22O11	342.3	0.135	Test set 2	351.1	1.427	1.378	1.548
					351.2	1.427	1.379	1.548
					351.4	1.427	1.380	1.549
					351.5	1.427	1.380	1.550
					351.7	1.427	1.381	1.550
					351.8	1.428	1.381	1.551
					352.0	1.429	1.382	1.551
					352.1	1.429	1.383	1.552
					352.3	1.431	1.383	1.552
					352.4	1.432	1.384	1.553
					352.6	1.432	1.384	1.554
					352.7	1.434	1.385	1.554
					352.9	1.434	1.386	1.555
					353.0	1.435	1.386	1.555
					353.2	1.435	1.387	1.556

					353.3	1.435	1.387	1.557
					353.5	1.437	1.388	1.557
					353.6	1.437	1.388	1.558
					353.8	1.437	1.389	1.558
					353.9	1.436	1.390	1.559
					354.1	1.437	1.390	1.560
					354.2	1.436	1.391	1.560
					354.4	1.438	1.391	1.561
					354.5	1.439	1.392	1.561
					354.7	1.440	1.393	1.562
					354.8	1.441	1.393	1.562
					355.0	1.442	1.394	1.563
					355.2	1.442	1.394	1.564
					355.3	1.443	1.395	1.564
					355.5	1.444	1.396	1.565
					355.6	1.445	1.396	1.565
					355.8	1.446	1.397	1.566
					355.9	1.446	1.397	1.567

					356.1	1.446	1.398	1.567
					356.2	1.448	1.399	1.568
Maltose	C12H22O11	342.3	0.135	Test set 2	356.4	1.448	1.399	1.568
					356.5	1.448	1.400	1.569
					356.7	1.449	1.400	1.570
					356.8	1.451	1.401	1.570
					357.0	1.453	1.401	1.571
					357.1	1.453	1.402	1.571
					357.3	1.453	1.403	1.572
					357.4	1.454	1.403	1.573
					357.6	1.455	1.404	1.573
					357.7	1.456	1.404	1.574
					357.9	1.456	1.405	1.574
					358.0	1.457	1.406	1.575
					358.2	1.459	1.406	1.576
					358.3	1.460	1.407	1.576
					358.5	1.461	1.407	1.577
					358.6	1.463	1.408	1.577

					358.8	1.464	1.409	1.578
					358.9	1.464	1.409	1.578
					359.1	1.465	1.410	1.579
					359.2	1.466	1.410	1.580
					359.4	1.467	1.411	1.580
					359.5	1.467	1.412	1.581
					359.7	1.468	1.412	1.581
					359.8	1.469	1.413	1.582
					360.0	1.469	1.413	1.583
					360.1	1.470	1.414	1.583
					360.3	1.472	1.414	1.584
					360.4	1.472	1.415	1.584
					360.6	1.471	1.416	1.585
					360.7	1.472	1.416	1.586
					360.9	1.473	1.417	1.586
					361.0	1.473	1.417	1.587
					361.2	1.475	1.418	1.587
					361.3	1.477	1.419	1.588

					361.5	1.477	1.419	1.589
Maltose	C12H22O11	342.3	0.135	Test set 2	361.6	1.479	1.420	1.589
					361.8	1.479	1.420	1.590
					361.9	1.480	1.421	1.590
					362.1	1.482	1.422	1.591
					362.2	1.484	1.422	1.591
					362.4	1.484	1.423	1.592
					362.5	1.484	1.423	1.593
					362.7	1.487	1.424	1.593
					362.8	1.487	1.425	1.594
					363.0	1.488	1.425	1.594
					363.1	1.490	1.426	1.595
					363.3	1.491	1.426	1.596
					363.4	1.494	1.427	1.596
					363.6	1.494	1.427	1.597
					363.7	1.495	1.428	1.597
					363.9	1.497	1.429	1.598
					364.0	1.497	1.429	1.599

					364.2	1.498	1.430	1.599
					364.3	1.498	1.430	1.600
					364.5	1.497	1.431	1.600
					364.6	1.499	1.432	1.601
					364.8	1.499	1.432	1.602
					364.9	1.500	1.433	1.602
					365.1	1.499	1.433	1.603
					365.2	1.500	1.434	1.603
					365.4	1.501	1.435	1.604
					365.5	1.501	1.435	1.605
					365.7	1.502	1.436	1.605
					365.8	1.504	1.436	1.606
					366.0	1.506	1.437	1.606
					366.1	1.508	1.438	1.607
					366.3	1.509	1.438	1.607
					366.4	1.510	1.439	1.608
					366.6	1.510	1.439	1.609
					366.7	1.511	1.440	1.609

Maltose	C12H22O11	342.3	0.135	Test set 2	366.9	1.512	1.441	1.610
					367.0	1.512	1.441	1.610
					367.2	1.512	1.442	1.611
					367.3	1.514	1.442	1.612
					367.5	1.516	1.443	1.612
					367.6	1.518	1.443	1.613
					367.8	1.519	1.444	1.613
					367.9	1.522	1.445	1.614
					368.1	1.525	1.445	1.615
					368.2	1.527	1.446	1.615
					368.4	1.528	1.446	1.616
					368.5	1.530	1.447	1.616
					368.7	1.531	1.448	1.617
					368.8	1.532	1.448	1.618
					369.0	1.534	1.449	1.618
					369.1	1.535	1.449	1.619
					369.3	1.538	1.450	1.619
					369.4	1.538	1.451	1.620

					369.6	1.539	1.451	1.621
					369.7	1.539	1.452	1.621
					369.9	1.540	1.452	1.622
					370.0	1.541	1.453	1.622
					370.2	1.543	1.454	1.623
					370.3	1.544	1.454	1.623
					370.5	1.546	1.455	1.624
					370.6	1.546	1.455	1.625
					370.8	1.548	1.456	1.625
					370.9	1.548	1.457	1.626
					371.1	1.550	1.457	1.626
					371.2	1.550	1.458	1.627
					371.4	1.553	1.458	1.628
					371.5	1.554	1.459	1.628
					371.7	1.555	1.460	1.629
					371.8	1.556	1.460	1.629
					372.0	1.558	1.461	1.630
Maltose	C12H22O11	342.3	0.135	Test set 2	372.1	1.559	1.461	1.631

					372.3	1.561	1.462	1.631
					372.4	1.563	1.462	1.632
					372.6	1.566	1.463	1.632
					372.7	1.568	1.464	1.633
					372.9	1.569	1.464	1.634
					373.0	1.570	1.465	1.634
					373.2	1.573	1.465	1.635
					373.3	1.576	1.466	1.635
					373.5	1.577	1.467	1.636
					373.6	1.580	1.467	1.637
					373.8	1.581	1.468	1.637
					373.9	1.582	1.468	1.638
					374.1	1.583	1.469	1.638
					374.2	1.585	1.470	1.639
					374.4	1.585	1.470	1.640
					374.5	1.586	1.471	1.640
					374.7	1.587	1.471	1.641
					374.8	1.589	1.472	1.641

					375.0	1.589	1.473	1.642
					375.1	1.592	1.473	1.642
					375.3	1.595	1.474	1.643
					375.4	1.598	1.474	1.644
					375.6	1.599	1.475	1.644
					375.7	1.602	1.476	1.645
					375.9	1.604	1.476	1.645
					376.0	1.607	1.477	1.646
					376.2	1.609	1.477	1.647
					376.3	1.611	1.478	1.647
					376.5	1.613	1.479	1.648
					376.6	1.616	1.479	1.648
					376.8	1.618	1.480	1.649
					376.9	1.620	1.480	1.650
					377.1	1.625	1.481	1.650
					377.2	1.628	1.482	1.651
Maltose	C12H22O11	342.3	0.135	Test set 2	377.4	1.631	1.482	1.651
					377.5	1.636	1.483	1.652

					377.7	1.638	1.483	1.653
					377.8	1.640	1.484	1.653
					378.0	1.644	1.484	1.654
					378.1	1.646	1.485	1.654
					378.3	1.649	1.486	1.655
					378.4	1.652	1.486	1.656
					378.6	1.655	1.487	1.656
					378.7	1.657	1.487	1.657
					378.9	1.659	1.488	1.657
					379.0	1.662	1.489	1.658
					379.2	1.664	1.489	1.659
					379.3	1.668	1.490	1.659
					379.5	1.672	1.490	1.660
					379.6	1.676	1.491	1.660
					379.8	1.680	1.492	1.661
					379.9	1.684	1.492	1.662
					380.1	1.688	1.493	1.662
					380.2	1.692	1.493	1.663

					380.4	1.695	1.494	1.663
					380.5	1.698	1.495	1.664
					380.7	1.701	1.495	1.665
					380.8	1.702	1.496	1.665
					381.0	1.704	1.496	1.666
					381.1	1.706	1.497	1.666
					381.3	1.709	1.498	1.667
					381.4	1.713	1.498	1.667
					381.6	1.717	1.499	1.668
					381.7	1.719	1.499	1.669
					381.9	1.725	1.500	1.669
					382.0	1.729	1.501	1.670
					382.2	1.733	1.501	1.670
					382.3	1.738	1.502	1.671
					382.5	1.742	1.502	1.672
					382.6	1.747	1.503	1.672
					382.8	1.750	1.504	1.673
					382.9	1.755	1.504	1.673

					383.1	1.758	1.505	1.674
					383.2	1.762	1.505	1.675
					383.4	1.765	1.506	1.675
					383.5	1.768	1.507	1.676
					383.7	1.771	1.507	1.676
					383.8	1.774	1.508	1.677
					384.0	1.777	1.508	1.678
					384.1	1.780	1.509	1.678
					384.3	1.783	1.510	1.679
					384.4	1.787	1.510	1.679
					384.6	1.792	1.511	1.680
					384.7	1.797	1.511	1.681
					384.9	1.803	1.512	1.681
					385.0	1.808	1.513	1.682
Trehalose	C12H22O11	342.3	0.135	Test set 2	323.2	1.400	1.282	1.457
					323.3	1.401	1.283	1.457
					323.4	1.400	1.283	1.458
					323.6	1.399	1.284	1.458

					323.7	1.400	1.284	1.459
					323.8	1.400	1.285	1.459
					323.9	1.400	1.285	1.460
					324.0	1.401	1.285	1.460
					324.1	1.401	1.286	1.461
					324.3	1.403	1.286	1.461
					324.4	1.401	1.287	1.461
					324.5	1.401	1.287	1.462
					324.6	1.402	1.288	1.462
					324.7	1.400	1.288	1.463
					324.8	1.400	1.289	1.463
					325.0	1.400	1.289	1.464
					325.1	1.401	1.290	1.464
					325.2	1.401	1.290	1.465
Trehalose	C12H22O11	342.3	0.135	Test set 2	325.3	1.404	1.290	1.465
					325.4	1.405	1.291	1.466
					325.5	1.404	1.291	1.466
					325.7	1.404	1.292	1.466

					325.8	1.406	1.292	1.467
					325.9	1.404	1.293	1.467
					326.0	1.404	1.293	1.468
					326.1	1.404	1.294	1.468
					326.2	1.406	1.294	1.469
					326.4	1.404	1.294	1.469
					326.5	1.406	1.295	1.470
					326.6	1.408	1.295	1.470
					326.7	1.409	1.296	1.470
					326.8	1.409	1.296	1.471
					326.9	1.409	1.297	1.471
					327.1	1.410	1.297	1.472
					327.2	1.412	1.298	1.472
					327.3	1.413	1.298	1.473
					327.4	1.413	1.299	1.473
					327.5	1.415	1.299	1.474
					327.6	1.415	1.299	1.474
					327.8	1.416	1.300	1.475

					327.9	1.416	1.300	1.475
					328.0	1.415	1.301	1.475
					328.1	1.415	1.301	1.476
					328.2	1.417	1.302	1.476
					328.3	1.418	1.302	1.477
					328.4	1.417	1.303	1.477
					328.6	1.417	1.303	1.478
					328.7	1.417	1.303	1.478
					328.8	1.417	1.304	1.479
					328.9	1.419	1.304	1.479
					329.0	1.418	1.305	1.480
					329.1	1.418	1.305	1.480
					329.3	1.417	1.306	1.480
Trehalose	C12H22O11	342.3	0.135	Test set 2	329.4	1.420	1.306	1.481
					329.5	1.420	1.307	1.481
					329.6	1.422	1.307	1.482
					329.7	1.422	1.308	1.482
					329.8	1.422	1.308	1.483

					330.0	1.423	1.308	1.483
					330.1	1.423	1.309	1.484
					330.2	1.425	1.309	1.484
					330.3	1.425	1.310	1.484
					330.4	1.427	1.310	1.485
					330.5	1.430	1.311	1.485
					330.6	1.430	1.311	1.486
					330.8	1.431	1.312	1.486
					330.9	1.430	1.312	1.487
					331.0	1.430	1.312	1.487
					331.1	1.429	1.313	1.488
					331.2	1.428	1.313	1.488
					331.3	1.428	1.314	1.489
					331.5	1.428	1.314	1.489
					331.6	1.429	1.315	1.489
					331.7	1.429	1.315	1.490
					331.8	1.429	1.316	1.490
					331.9	1.431	1.316	1.491

					332.0	1.431	1.317	1.491
					332.2	1.431	1.317	1.492
					332.3	1.432	1.317	1.492
					332.4	1.433	1.318	1.493
					332.5	1.431	1.318	1.493
					332.6	1.433	1.319	1.493
					332.7	1.434	1.319	1.494
					332.8	1.434	1.320	1.494
					333.0	1.437	1.320	1.495
					333.1	1.437	1.321	1.495
					333.2	1.439	1.321	1.496
					333.3	1.440	1.321	1.496
Trehalose	C12H22O11	342.3	0.135	Test set 2	333.4	1.440	1.322	1.497
					333.5	1.442	1.322	1.497
					333.7	1.441	1.323	1.498
					333.8	1.441	1.323	1.498
					333.9	1.442	1.324	1.498
					334.0	1.444	1.324	1.499

					334.1	1.443	1.325	1.499
					334.2	1.444	1.325	1.500
					334.3	1.445	1.326	1.500
					334.5	1.445	1.326	1.501
					334.6	1.445	1.326	1.501
					334.7	1.447	1.327	1.502
					334.8	1.447	1.327	1.502
					334.9	1.447	1.328	1.502
					335.0	1.447	1.328	1.503
					335.2	1.447	1.329	1.503
					335.3	1.449	1.329	1.504
					335.4	1.449	1.330	1.504
					335.5	1.449	1.330	1.505
					335.6	1.452	1.330	1.505
					335.7	1.454	1.331	1.506
					335.8	1.454	1.331	1.506
					336.0	1.453	1.332	1.507
					336.1	1.454	1.332	1.507

					336.2	1.452	1.333	1.507
					336.3	1.452	1.333	1.508
					336.4	1.451	1.334	1.508
					336.5	1.451	1.334	1.509
					336.7	1.453	1.335	1.509
					336.8	1.454	1.335	1.510
					336.9	1.453	1.335	1.510
					337.0	1.456	1.336	1.511
					337.1	1.455	1.336	1.511
					337.2	1.457	1.337	1.511
					337.3	1.456	1.337	1.512
Trehalose	C12H22O11	342.3	0.135	Test set 2	337.5	1.456	1.338	1.512
					337.6	1.457	1.338	1.513
					337.7	1.457	1.339	1.513
					337.8	1.458	1.339	1.514
					337.9	1.459	1.340	1.514
					338.0	1.460	1.340	1.515
					338.2	1.459	1.340	1.515

					338.3	1.461	1.341	1.516
					338.4	1.464	1.341	1.516
					338.5	1.464	1.342	1.516
					338.6	1.464	1.342	1.517
					338.7	1.464	1.343	1.517
					338.8	1.465	1.343	1.518
					339.0	1.466	1.344	1.518
					339.1	1.466	1.344	1.519
					339.2	1.467	1.344	1.519
					339.3	1.467	1.345	1.520
					339.4	1.467	1.345	1.520
					339.5	1.469	1.346	1.520
					339.7	1.468	1.346	1.521
					339.8	1.469	1.347	1.521
					339.9	1.468	1.347	1.522
					340.0	1.467	1.348	1.522
					340.1	1.467	1.348	1.523
					340.2	1.469	1.349	1.523

					340.3	1.467	1.349	1.524
					340.5	1.469	1.349	1.524
					340.6	1.468	1.350	1.525
					340.7	1.469	1.350	1.525
					340.8	1.467	1.351	1.525
					340.9	1.467	1.351	1.526
					341.0	1.468	1.352	1.526
					341.2	1.470	1.352	1.527
					341.3	1.471	1.353	1.527
					341.4	1.473	1.353	1.528
Trehalose	C12H22O11	342.3	0.135	Test set 2	341.5	1.475	1.354	1.528
					341.6	1.474	1.354	1.529
					341.7	1.475	1.354	1.529
					341.8	1.476	1.355	1.529
					342.0	1.477	1.355	1.530
					342.1	1.478	1.356	1.530
					342.2	1.479	1.356	1.531
					342.3	1.479	1.357	1.531

					342.4	1.479	1.357	1.532
					342.5	1.479	1.358	1.532
					342.7	1.480	1.358	1.533
					342.8	1.479	1.358	1.533
					342.9	1.480	1.359	1.534
					343.0	1.481	1.359	1.534
					343.1	1.482	1.360	1.534
					343.2	1.485	1.360	1.535
					343.3	1.484	1.361	1.535
					343.5	1.484	1.361	1.536
					343.6	1.486	1.362	1.536
					343.7	1.484	1.362	1.537
					343.8	1.485	1.363	1.537
					343.9	1.485	1.363	1.538
					344.0	1.486	1.363	1.538
					344.2	1.486	1.364	1.539
					344.3	1.486	1.364	1.539
					344.4	1.488	1.365	1.539

					344.5	1.487	1.365	1.540
					344.6	1.487	1.366	1.540
					344.7	1.487	1.366	1.541
					344.8	1.487	1.367	1.541
					345.0	1.489	1.367	1.542
					345.1	1.492	1.367	1.542
					345.2	1.493	1.368	1.543
					345.3	1.492	1.368	1.543
					345.4	1.495	1.369	1.543
Trehalose	C12H22O11	342.3	0.135	Test set 2	345.5	1.497	1.369	1.544
					345.6	1.498	1.370	1.544
					345.8	1.498	1.370	1.545
					345.9	1.497	1.371	1.545
					346.0	1.500	1.371	1.546
					346.1	1.500	1.372	1.546
					346.2	1.501	1.372	1.547
					346.3	1.501	1.372	1.547
					346.5	1.502	1.373	1.548

					346.6	1.502	1.373	1.548
					346.7	1.503	1.374	1.548
					346.8	1.501	1.374	1.549
					346.9	1.502	1.375	1.549
					347.0	1.502	1.375	1.550
					347.1	1.502	1.376	1.550
					347.3	1.503	1.376	1.551
					347.4	1.501	1.377	1.551
					347.5	1.503	1.377	1.552
					347.6	1.506	1.377	1.552
					347.7	1.506	1.378	1.553
					347.8	1.509	1.378	1.553
					347.9	1.510	1.379	1.553
					348.1	1.513	1.379	1.554
					348.2	1.513	1.380	1.554
					348.3	1.513	1.380	1.555
					348.4	1.514	1.381	1.555
					348.5	1.513	1.381	1.556

					348.6	1.514	1.381	1.556
					348.8	1.514	1.382	1.557
					348.9	1.513	1.382	1.557
					349.0	1.515	1.383	1.557
					349.1	1.516	1.383	1.558
					349.2	1.514	1.384	1.558
					349.3	1.511	1.384	1.559
					349.4	1.511	1.385	1.559
Trehalose	C12H22O11	342.3	0.135	Test set 2	349.6	1.513	1.385	1.560
					349.7	1.511	1.386	1.560
					349.8	1.511	1.386	1.561
					349.9	1.510	1.386	1.561
					350.0	1.511	1.387	1.562
					350.1	1.512	1.387	1.562
					350.3	1.513	1.388	1.562
					350.4	1.514	1.388	1.563
					350.5	1.514	1.389	1.563
					350.6	1.514	1.389	1.564

					350.7	1.515	1.390	1.564
					350.8	1.515	1.390	1.565
					350.9	1.515	1.391	1.565
					351.1	1.517	1.391	1.566
					351.2	1.518	1.391	1.566
					351.3	1.520	1.392	1.567
					351.4	1.524	1.392	1.567
					351.5	1.523	1.393	1.567
					351.6	1.525	1.393	1.568
					351.7	1.525	1.394	1.568
					351.9	1.525	1.394	1.569
					352.0	1.525	1.395	1.569
					352.1	1.524	1.395	1.570
					352.2	1.523	1.395	1.570
					352.3	1.524	1.396	1.571
					352.4	1.524	1.396	1.571
					352.5	1.523	1.397	1.571
					352.7	1.526	1.397	1.572

					352.8	1.527	1.398	1.572
					352.9	1.529	1.398	1.573
					353.0	1.531	1.399	1.573
					353.1	1.533	1.399	1.574
					353.2	1.532	1.400	1.574
					353.4	1.532	1.400	1.575
					353.5	1.534	1.400	1.575
Trehalose	C12H22O11	342.3	0.135	Test set 2	353.6	1.534	1.401	1.576
					353.7	1.534	1.401	1.576
					353.8	1.535	1.402	1.576
					353.9	1.536	1.402	1.577
					354.0	1.537	1.403	1.577
					354.2	1.538	1.403	1.578
					354.3	1.539	1.404	1.578
					354.4	1.542	1.404	1.579
					354.5	1.544	1.405	1.579
					354.6	1.544	1.405	1.580
					354.7	1.545	1.405	1.580

					354.8	1.545	1.406	1.581
					355.0	1.545	1.406	1.581
					355.1	1.543	1.407	1.581
					355.2	1.544	1.407	1.582
					355.3	1.545	1.408	1.582
					355.4	1.546	1.408	1.583
					355.5	1.546	1.409	1.583
					355.7	1.545	1.409	1.584
					355.8	1.544	1.410	1.584
					355.9	1.545	1.410	1.585
					356.0	1.546	1.410	1.585
Galactose	C6H12O6	180.2	0.133	Test set 2	332.9	1.393	1.308	1.477
					333.1	1.394	1.308	1.478
					333.2	1.394	1.309	1.478
					333.4	1.394	1.310	1.479
					333.6	1.394	1.310	1.480
					333.7	1.393	1.311	1.480
					333.9	1.393	1.312	1.481

					334.0	1.393	1.312	1.481
					334.2	1.393	1.313	1.482
					334.4	1.393	1.313	1.483
					334.5	1.392	1.314	1.483
					334.7	1.392	1.315	1.484
					334.8	1.393	1.315	1.485
Galactose	C6H12O6	180.2	0.133	Test set 2	335.0	1.393	1.316	1.485
					335.2	1.394	1.316	1.486
					335.3	1.395	1.317	1.486
					335.5	1.395	1.318	1.487
					335.7	1.395	1.318	1.488
					335.8	1.395	1.319	1.488
					336.0	1.397	1.320	1.489
					336.1	1.398	1.320	1.490
					336.3	1.399	1.321	1.490
					336.5	1.400	1.322	1.491
					336.6	1.400	1.322	1.491
					336.8	1.401	1.323	1.492

					336.9	1.402	1.323	1.493
					337.1	1.402	1.324	1.493
					337.3	1.401	1.325	1.494
					337.4	1.402	1.325	1.495
					337.6	1.402	1.326	1.495
					337.7	1.403	1.326	1.496
					337.9	1.403	1.327	1.496
					338.1	1.404	1.328	1.497
					338.2	1.405	1.328	1.498
					338.4	1.406	1.329	1.498
					338.5	1.406	1.330	1.499
					338.7	1.407	1.330	1.499
					338.9	1.408	1.331	1.500
					339.0	1.409	1.331	1.501
					339.2	1.410	1.332	1.501
					339.3	1.410	1.333	1.502
					339.5	1.411	1.333	1.503
					339.7	1.413	1.334	1.503

					339.8	1.413	1.335	1.504
					340.0	1.414	1.335	1.504
					340.1	1.415	1.336	1.505
					340.3	1.417	1.336	1.506
					340.5	1.418	1.337	1.506
Galactose	C6H12O6	180.2	0.133	Test set 2	340.6	1.419	1.338	1.507
					340.8	1.420	1.338	1.508
					340.9	1.421	1.339	1.508
					341.1	1.422	1.340	1.509
					341.3	1.423	1.340	1.509
					341.4	1.425	1.341	1.510
					341.6	1.426	1.341	1.511
					341.7	1.428	1.342	1.511
					341.9	1.429	1.343	1.512
					342.1	1.430	1.343	1.513
					342.2	1.431	1.344	1.513
					342.4	1.432	1.345	1.514
					342.5	1.434	1.345	1.514

					342.7	1.435	1.346	1.515
					342.9	1.435	1.346	1.516
					343.0	1.435	1.347	1.516
					343.2	1.435	1.348	1.517
					343.3	1.436	1.348	1.518
					343.5	1.437	1.349	1.518
					343.7	1.438	1.349	1.519
					343.8	1.438	1.350	1.519
					344.0	1.438	1.351	1.520
					344.1	1.439	1.351	1.521
					344.3	1.438	1.352	1.521
					344.5	1.438	1.353	1.522
					344.6	1.438	1.353	1.523
					344.8	1.439	1.354	1.523
					344.9	1.439	1.354	1.524
					345.1	1.439	1.355	1.524
					345.3	1.440	1.356	1.525
					345.4	1.442	1.356	1.526

					345.6	1.442	1.357	1.526
					345.7	1.443	1.358	1.527
					345.9	1.444	1.358	1.528
					346.1	1.446	1.359	1.528
Galactose	C6H12O6	180.2	0.133	Test set 2	346.2	1.448	1.359	1.529
					346.4	1.449	1.360	1.529
					346.5	1.450	1.361	1.530
					346.7	1.452	1.361	1.531
					346.9	1.454	1.362	1.531
					347.0	1.455	1.363	1.532
					347.2	1.456	1.363	1.532
					347.3	1.456	1.364	1.533
					347.5	1.457	1.364	1.534
					347.6	1.457	1.365	1.534
					347.8	1.458	1.366	1.535
					348.0	1.459	1.366	1.536
					348.1	1.460	1.367	1.536
					348.3	1.460	1.368	1.537

					348.4	1.461	1.368	1.537
					348.6	1.461	1.369	1.538
					348.8	1.461	1.369	1.539
					348.9	1.460	1.370	1.539
					349.1	1.460	1.371	1.540
					349.2	1.461	1.371	1.541
					349.4	1.461	1.372	1.541
					349.6	1.462	1.373	1.542
					349.7	1.463	1.373	1.542
					349.9	1.463	1.374	1.543
					350.0	1.464	1.374	1.544
					350.2	1.465	1.375	1.544
					350.4	1.465	1.376	1.545
					350.5	1.466	1.376	1.546
					350.7	1.466	1.377	1.546
					350.8	1.466	1.378	1.547
					351.0	1.466	1.378	1.547
					351.2	1.466	1.379	1.548

					351.3	1.466	1.379	1.549
					351.5	1.466	1.380	1.549
					351.6	1.465	1.381	1.550
Galactose	C6H12O6	180.2	0.133	Test set 2	351.8	1.465	1.381	1.551
					352.0	1.465	1.382	1.551
					352.1	1.465	1.383	1.552
					352.3	1.466	1.383	1.552
					352.4	1.466	1.384	1.553
					352.6	1.467	1.384	1.554
					352.8	1.469	1.385	1.554
					352.9	1.470	1.386	1.555
					353.1	1.469	1.386	1.556
					353.2	1.468	1.387	1.556
					353.4	1.468	1.387	1.557
					353.5	1.469	1.388	1.557
					353.7	1.470	1.389	1.558
					353.9	1.470	1.389	1.559
					354.0	1.472	1.390	1.559

					354.2	1.473	1.391	1.560
					354.3	1.473	1.391	1.561
					354.5	1.474	1.392	1.561
					354.7	1.475	1.392	1.562
					354.8	1.476	1.393	1.562
					355.0	1.477	1.394	1.563
					355.1	1.478	1.394	1.564
					355.3	1.480	1.395	1.564
					355.5	1.481	1.396	1.565
					355.6	1.483	1.396	1.566
					355.8	1.485	1.397	1.566
					355.9	1.487	1.397	1.567
					356.1	1.488	1.398	1.567
					356.3	1.489	1.399	1.568
					356.4	1.490	1.399	1.569
					356.6	1.491	1.400	1.569
					356.7	1.493	1.401	1.570
					356.9	1.494	1.401	1.570

					357.0	1.496	1.402	1.571
					357.2	1.497	1.402	1.572
Galactose	C6H12O6	180.2	0.133	Test set 2	357.4	1.499	1.403	1.572
					357.5	1.501	1.404	1.573
					357.7	1.502	1.404	1.574
					357.8	1.504	1.405	1.574
					358.0	1.506	1.406	1.575
					358.2	1.508	1.406	1.576
					358.3	1.510	1.407	1.576
					358.5	1.511	1.407	1.577
					358.6	1.511	1.408	1.577
					358.8	1.511	1.409	1.578
					359.0	1.511	1.409	1.579
					359.1	1.510	1.410	1.579
					359.3	1.510	1.411	1.580
					359.4	1.510	1.411	1.580
					359.6	1.510	1.412	1.581
					359.7	1.510	1.412	1.582

					359.9	1.511	1.413	1.582
					360.1	1.512	1.414	1.583
					360.2	1.513	1.414	1.584
					360.4	1.514	1.415	1.584
					360.5	1.515	1.416	1.585
					360.7	1.515	1.416	1.585
					360.9	1.516	1.417	1.586
					361.0	1.517	1.417	1.587
					361.2	1.518	1.418	1.587
					361.3	1.518	1.419	1.588
					361.5	1.517	1.419	1.589
					361.7	1.517	1.420	1.589
					361.8	1.517	1.421	1.590
					362.0	1.518	1.421	1.590
					362.1	1.520	1.422	1.591
					362.3	1.521	1.422	1.592
					362.5	1.523	1.423	1.592
					362.6	1.524	1.424	1.593

					362.8	1.523	1.424	1.594
Galactose	C6H12O6	180.2	0.133	Test set 2	362.9	1.523	1.425	1.594
					363.1	1.523	1.426	1.595
					363.2	1.524	1.426	1.595
					363.4	1.524	1.427	1.596
					363.6	1.524	1.427	1.597
					363.7	1.524	1.428	1.597
					363.9	1.525	1.429	1.598
					364.0	1.525	1.429	1.599
					364.2	1.526	1.430	1.599
					364.4	1.528	1.431	1.600
					364.5	1.529	1.431	1.600
					364.7	1.529	1.432	1.601
					364.8	1.530	1.432	1.602
					365.0	1.531	1.433	1.602
					365.1	1.532	1.434	1.603
					365.3	1.533	1.434	1.604
					365.5	1.535	1.435	1.604

					365.6	1.536	1.436	1.605
					365.8	1.537	1.436	1.605
					365.9	1.538	1.437	1.606
					366.1	1.539	1.437	1.607
					366.3	1.541	1.438	1.607
					366.4	1.542	1.439	1.608
					366.6	1.542	1.439	1.609
					366.7	1.541	1.440	1.609
					366.9	1.540	1.441	1.610
					367.1	1.540	1.441	1.610
					367.2	1.539	1.442	1.611
					367.4	1.539	1.442	1.612
					367.5	1.537	1.443	1.612
					367.7	1.536	1.444	1.613
					367.8	1.536	1.444	1.614
					368.0	1.537	1.445	1.614
					368.2	1.537	1.446	1.615
					368.3	1.537	1.446	1.616

Galactose	C6H12O6	180.2	0.133	Test set 2	368.5	1.537	1.447	1.616
					368.6	1.538	1.447	1.617
					368.8	1.539	1.448	1.617
					369.0	1.539	1.449	1.618
					369.1	1.541	1.449	1.619
					369.3	1.542	1.450	1.619
					369.4	1.543	1.451	1.620
					369.6	1.544	1.451	1.620
					369.7	1.544	1.452	1.621
					369.9	1.544	1.452	1.622
					370.1	1.544	1.453	1.622
					370.2	1.545	1.454	1.623
					370.4	1.546	1.454	1.624
					370.5	1.547	1.455	1.624
					370.7	1.547	1.456	1.625
					370.9	1.548	1.456	1.626
					371.0	1.547	1.457	1.626
					371.2	1.547	1.457	1.627

					371.3	1.548	1.458	1.627
					371.5	1.547	1.459	1.628
					371.7	1.546	1.459	1.629
					371.8	1.546	1.460	1.629
					372.0	1.546	1.461	1.630
					372.1	1.547	1.461	1.631
					372.3	1.548	1.462	1.631
					372.4	1.549	1.462	1.632
					372.6	1.549	1.463	1.632
					372.8	1.550	1.464	1.633
					372.9	1.550	1.464	1.634
					373.1	1.551	1.465	1.634
					373.2	1.551	1.466	1.635
					373.4	1.551	1.466	1.636
					373.6	1.551	1.467	1.636
					373.7	1.551	1.468	1.637
					373.9	1.552	1.468	1.637
Galactose	C6H12O6	180.2	0.133	Test set 2	374.0	1.552	1.469	1.638

					374.2	1.553	1.469	1.639
					374.3	1.553	1.470	1.639
					374.5	1.553	1.471	1.640
					374.7	1.553	1.471	1.641
					374.8	1.554	1.472	1.641
					375.0	1.554	1.473	1.642
					375.1	1.553	1.473	1.642
					375.3	1.554	1.474	1.643
					375.5	1.555	1.474	1.644
					375.6	1.556	1.475	1.644
					375.8	1.557	1.476	1.645
					375.9	1.558	1.476	1.646
					376.1	1.558	1.477	1.646
					376.3	1.558	1.478	1.647
					376.4	1.559	1.478	1.647
					376.6	1.560	1.479	1.648
					376.7	1.560	1.479	1.649
					376.9	1.559	1.480	1.649

					377.0	1.558	1.481	1.650
					377.2	1.556	1.481	1.651
					377.4	1.556	1.482	1.651
					377.5	1.558	1.483	1.652
					377.7	1.560	1.483	1.653
					377.8	1.568	1.484	1.653
					378.0	1.570	1.484	1.654
					378.1	1.569	1.485	1.654
					378.3	1.568	1.486	1.655
					378.5	1.566	1.486	1.656
					378.6	1.566	1.487	1.656
					378.8	1.565	1.488	1.657
					378.9	1.564	1.488	1.658
					379.1	1.563	1.489	1.658
					379.3	1.565	1.490	1.659
					379.4	1.567	1.490	1.659
Galactose	C6H12O6	180.2	0.133	Test set 2	379.6	1.569	1.491	1.660
					379.7	1.572	1.491	1.661

					379.9	1.575	1.492	1.661
					380.1	1.577	1.493	1.662
					380.2	1.579	1.493	1.663
					380.4	1.581	1.494	1.663
					380.5	1.582	1.495	1.664
					380.7	1.584	1.495	1.664
					380.8	1.585	1.496	1.665
					381.0	1.585	1.496	1.666
					381.2	1.585	1.497	1.666
					381.3	1.586	1.498	1.667
					381.5	1.587	1.498	1.668
					381.6	1.588	1.499	1.668
					381.8	1.589	1.500	1.669
					382.0	1.590	1.500	1.670
					382.1	1.590	1.501	1.670
					382.3	1.590	1.501	1.671
					382.4	1.590	1.502	1.671
					382.6	1.590	1.503	1.672

					382.7	1.591	1.503	1.673
					382.9	1.592	1.504	1.673
					383.1	1.592	1.505	1.674
					383.2	1.594	1.505	1.675
					383.4	1.595	1.506	1.675
					383.5	1.595	1.507	1.676
					383.7	1.596	1.507	1.676
					383.9	1.596	1.508	1.677
					384.0	1.598	1.508	1.678
					384.2	1.599	1.509	1.678
					384.3	1.600	1.510	1.679
					384.5	1.600	1.510	1.680
					384.6	1.600	1.511	1.680
					384.8	1.600	1.512	1.681
					385.0	1.601	1.512	1.681
Galactose	C6H12O6	180.2	0.133	Test set 2	385.1	1.603	1.513	1.682
					385.3	1.604	1.513	1.683
					385.4	1.605	1.514	1.683

					385.6	1.606	1.515	1.684
					385.8	1.606	1.515	1.685
					385.9	1.606	1.516	1.685
					386.1	1.607	1.517	1.686
					386.2	1.608	1.517	1.687
					386.4	1.608	1.518	1.687
					386.5	1.608	1.519	1.688
					386.7	1.608	1.519	1.688
					386.9	1.608	1.520	1.689
					387.0	1.608	1.520	1.690
					387.2	1.609	1.521	1.690
					387.3	1.609	1.522	1.691
					387.5	1.611	1.522	1.692
					387.6	1.611	1.523	1.692
					387.8	1.612	1.524	1.693
					388.0	1.613	1.524	1.693
					388.1	1.612	1.525	1.694
					388.3	1.611	1.525	1.695

					388.4	1.610	1.526	1.695
					388.6	1.610	1.527	1.696
					388.8	1.610	1.527	1.697
					388.9	1.610	1.528	1.697
					389.1	1.610	1.529	1.698
					389.2	1.610	1.529	1.699
					389.4	1.610	1.530	1.699
					389.5	1.610	1.530	1.700
					389.7	1.610	1.531	1.700
					389.9	1.611	1.532	1.701
					390.0	1.611	1.532	1.702
					390.2	1.610	1.533	1.702
					390.3	1.610	1.534	1.703
					390.5	1.611	1.534	1.704
Galactose	C6H12O6	180.2	0.133	Test set 2	390.7	1.612	1.535	1.704
					390.8	1.613	1.536	1.705
					391.0	1.612	1.536	1.705
					391.1	1.612	1.537	1.706

					391.3	1.613	1.537	1.707
					391.4	1.614	1.538	1.707
					391.6	1.615	1.539	1.708
					391.8	1.616	1.539	1.709
					391.9	1.617	1.540	1.709
					392.1	1.618	1.541	1.710
					392.2	1.620	1.541	1.711
					392.4	1.621	1.542	1.711
					392.6	1.621	1.543	1.712
					392.7	1.622	1.543	1.712
					392.9	1.622	1.544	1.713
					393.0	1.622	1.544	1.714
					393.2	1.621	1.545	1.714
					393.3	1.622	1.546	1.715
					393.5	1.623	1.546	1.716
					393.7	1.623	1.547	1.716
					393.8	1.624	1.548	1.717
					394.0	1.625	1.548	1.717

					394.1	1.625	1.549	1.718
					394.3	1.625	1.549	1.719
					394.5	1.625	1.550	1.719
					394.6	1.625	1.551	1.720
					394.8	1.625	1.551	1.721
					394.9	1.625	1.552	1.721
					395.1	1.626	1.553	1.722
					395.2	1.627	1.553	1.723
					395.4	1.626	1.554	1.723
					395.6	1.625	1.555	1.724
					395.7	1.625	1.555	1.724
					395.9	1.625	1.556	1.725
					396.0	1.625	1.556	1.726
Galactose	C6H12O6	180.2	0.133	Test set 2	396.2	1.625	1.557	1.726
					396.3	1.626	1.558	1.727
					396.5	1.626	1.558	1.728
					396.7	1.626	1.559	1.728
					396.8	1.628	1.560	1.729

					397.0	1.628	1.560	1.730
					397.1	1.629	1.561	1.730
					397.3	1.630	1.562	1.731
					397.5	1.631	1.562	1.731
					397.6	1.632	1.563	1.732
					397.8	1.633	1.563	1.733
					397.9	1.634	1.564	1.733
					398.1	1.635	1.565	1.734
					398.2	1.636	1.565	1.735
					398.4	1.638	1.566	1.735
					398.6	1.639	1.567	1.736
					398.7	1.641	1.567	1.737
					398.9	1.643	1.568	1.737
					399.0	1.646	1.569	1.738
					399.2	1.648	1.569	1.738
					399.4	1.649	1.570	1.739
					399.5	1.650	1.570	1.740
					399.7	1.650	1.571	1.740

					399.8	1.651	1.572	1.741
					400.0	1.651	1.572	1.742
					400.1	1.652	1.573	1.742
					400.3	1.653	1.574	1.743
					400.5	1.655	1.574	1.744
					400.6	1.656	1.575	1.744
					400.8	1.656	1.575	1.745
					400.9	1.657	1.576	1.745
					401.1	1.657	1.577	1.746
					401.3	1.657	1.577	1.747
					401.4	1.656	1.578	1.747
					401.6	1.657	1.579	1.748
Galactose	C6H12O6	180.2	0.133	Test set 2	401.7	1.658	1.579	1.749
					401.9	1.660	1.580	1.749
					402.0	1.661	1.581	1.750
					402.2	1.661	1.581	1.751
					402.4	1.660	1.582	1.751
					402.5	1.660	1.582	1.752

					402.7	1.660	1.583	1.752
					402.8	1.660	1.584	1.753
					403.0	1.660	1.584	1.754
					403.2	1.660	1.585	1.754
					403.3	1.662	1.586	1.755
					403.5	1.662	1.586	1.756
					403.6	1.664	1.587	1.756
					403.8	1.664	1.588	1.757
					403.9	1.664	1.588	1.757
					404.1	1.664	1.589	1.758
					404.3	1.664	1.589	1.759
					404.4	1.664	1.590	1.759
					404.6	1.664	1.591	1.760
					404.7	1.665	1.591	1.761
					404.9	1.666	1.592	1.761
					405.0	1.667	1.593	1.762
					405.2	1.667	1.593	1.763
					405.4	1.667	1.594	1.763

					405.5	1.668	1.595	1.764
					405.7	1.668	1.595	1.765
					405.8	1.669	1.596	1.765
					406.0	1.671	1.597	1.766
					406.2	1.672	1.597	1.766
					406.3	1.674	1.598	1.767
					406.5	1.675	1.598	1.768
					406.6	1.676	1.599	1.768
					406.8	1.677	1.600	1.769
					406.9	1.677	1.600	1.770
					407.1	1.678	1.601	1.770
Galactose	C6H12O6	180.2	0.133	Test set 2	407.3	1.679	1.602	1.771
					407.4	1.680	1.602	1.772
					407.6	1.682	1.603	1.772
					407.7	1.684	1.604	1.773
					407.9	1.685	1.604	1.773
					408.0	1.686	1.605	1.774
					408.2	1.687	1.605	1.775

					408.4	1.689	1.606	1.775
					408.5	1.690	1.607	1.776
					408.7	1.690	1.607	1.777
					408.8	1.690	1.608	1.777
					409.0	1.690	1.609	1.778
					409.2	1.690	1.609	1.779
					409.3	1.691	1.610	1.779
					409.5	1.692	1.611	1.780
					409.6	1.693	1.611	1.780
					409.8	1.695	1.612	1.781
					409.9	1.697	1.612	1.782
					410.1	1.698	1.613	1.782
					410.3	1.698	1.614	1.783
					410.4	1.696	1.614	1.784
					410.6	1.691	1.615	1.784
					410.7	1.688	1.616	1.785
					410.9	1.688	1.616	1.786
					411.1	1.689	1.617	1.786

					411.2	1.690	1.618	1.787
					411.4	1.691	1.618	1.787
					411.5	1.693	1.619	1.788
					411.7	1.695	1.619	1.789
					411.8	1.696	1.620	1.789
					412.0	1.695	1.621	1.790
					412.2	1.694	1.621	1.791
					412.3	1.694	1.622	1.791
					412.5	1.695	1.623	1.792
					412.6	1.696	1.623	1.793
Galactose	C6H12O6	180.2	0.133	Test set 2	412.8	1.696	1.624	1.793
					412.9	1.696	1.625	1.794
					413.1	1.696	1.625	1.795
					413.3	1.697	1.626	1.795
					413.4	1.697	1.627	1.796
					413.6	1.698	1.627	1.796
					413.7	1.699	1.628	1.797
					413.9	1.699	1.628	1.798

					414.1	1.700	1.629	1.798
					414.2	1.700	1.630	1.799
					414.4	1.701	1.630	1.800
					414.5	1.701	1.631	1.800
					414.7	1.702	1.632	1.801
					414.8	1.702	1.632	1.802
					415.0	1.703	1.633	1.802
					415.2	1.704	1.634	1.803
					415.3	1.703	1.634	1.803
					415.5	1.703	1.635	1.804
					415.6	1.703	1.635	1.805
					415.8	1.703	1.636	1.805
					416.0	1.704	1.637	1.806
					416.1	1.705	1.637	1.807
					416.3	1.707	1.638	1.807
					416.4	1.709	1.639	1.808
					416.6	1.710	1.639	1.809
					416.7	1.712	1.640	1.809

					416.9	1.713	1.641	1.810
					417.1	1.714	1.641	1.811
					417.2	1.714	1.642	1.811
					417.4	1.713	1.643	1.812
					417.5	1.713	1.643	1.812
					417.7	1.713	1.644	1.813
					417.8	1.713	1.644	1.814
					418.0	1.712	1.645	1.814
					418.2	1.711	1.646	1.815
Galactose	C6H12O6	180.2	0.133	Test set 2	418.3	1.711	1.646	1.816
					418.5	1.712	1.647	1.816
					418.6	1.712	1.648	1.817
					418.8	1.712	1.648	1.818
					419.0	1.713	1.649	1.818
					419.1	1.714	1.650	1.819
					419.3	1.715	1.650	1.820
					419.4	1.716	1.651	1.820
					419.6	1.717	1.652	1.821

					419.7	1.718	1.652	1.821
					419.9	1.719	1.653	1.822
					420.1	1.718	1.653	1.823
					420.2	1.719	1.654	1.823
					420.4	1.720	1.655	1.824
					420.5	1.721	1.655	1.825
					420.7	1.722	1.656	1.825
					420.9	1.722	1.657	1.826
					421.0	1.723	1.657	1.827
					421.2	1.725	1.658	1.827
					421.3	1.727	1.659	1.828
					421.5	1.726	1.659	1.829
					421.6	1.725	1.660	1.829
					421.8	1.723	1.660	1.830
					422.0	1.722	1.661	1.830
					422.1	1.720	1.662	1.831
					422.3	1.720	1.662	1.832
					422.4	1.724	1.663	1.832

					422.6	1.727	1.664	1.833
					422.7	1.729	1.664	1.834
					422.9	1.732	1.665	1.834
					423.1	1.734	1.666	1.835
					423.2	1.736	1.666	1.836
					423.4	1.737	1.667	1.836
					423.5	1.740	1.668	1.837
					423.7	1.743	1.668	1.838
Galactose	C6H12O6	180.2	0.133	Test set 2	423.9	1.745	1.669	1.838
					424.0	1.746	1.670	1.839
					424.2	1.748	1.670	1.839
					424.3	1.751	1.671	1.840
					424.5	1.753	1.671	1.841
					424.6	1.756	1.672	1.841
					424.8	1.760	1.673	1.842
					425.0	1.765	1.673	1.843
					425.1	1.768	1.674	1.843
					425.3	1.771	1.675	1.844

					425.4	1.774	1.675	1.845
					425.6	1.777	1.676	1.845
					425.7	1.779	1.677	1.846
					425.9	1.780	1.677	1.847
					426.1	1.781	1.678	1.847
					426.2	1.783	1.679	1.848
					426.4	1.786	1.679	1.848
					426.5	1.789	1.680	1.849
					426.7	1.792	1.680	1.850
					426.9	1.794	1.681	1.850
					427.0	1.797	1.682	1.851
					427.2	1.800	1.682	1.852
					427.3	1.804	1.683	1.852
					427.5	1.807	1.684	1.853
					427.6	1.811	1.684	1.854
					427.8	1.818	1.685	1.854
					428.0	1.824	1.686	1.855
					428.1	1.826	1.686	1.856

					428.3	1.834	1.687	1.856
					428.4	1.843	1.688	1.857
					428.6	1.850	1.688	1.857
					428.8	1.856	1.689	1.858
					428.9	1.863	1.690	1.859
					429.1	1.867	1.690	1.859
					429.2	1.868	1.691	1.860
					429.4	1.868	1.691	1.861
					429.5	1.870	1.692	1.861
					429.7	1.872	1.693	1.862
					429.9	1.876	1.693	1.863
					430.0	1.879	1.694	1.863
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	326.8	1.080	0.951	1.114
					326.9	1.083	0.952	1.115
					327.1	1.084	0.952	1.115
					327.3	1.086	0.953	1.116
					327.5	1.087	0.954	1.117
					327.6	1.087	0.954	1.117

					327.8	1.090	0.955	1.118
					328.0	1.091	0.955	1.118
					328.2	1.095	0.956	1.119
					328.4	1.095	0.956	1.119
					328.5	1.098	0.957	1.120
					328.7	1.098	0.957	1.120
					328.9	1.099	0.958	1.121
					329.1	1.101	0.959	1.122
					329.3	1.103	0.959	1.122
					329.4	1.105	0.960	1.123
					329.6	1.108	0.960	1.123
					329.8	1.110	0.961	1.124
					330.0	1.110	0.961	1.124
					330.1	1.110	0.962	1.125
					330.3	1.111	0.962	1.125
					330.5	1.109	0.963	1.126
					330.7	1.109	0.963	1.126
					330.9	1.111	0.964	1.127

					331.0	1.111	0.965	1.128
					331.2	1.113	0.965	1.128
					331.4	1.116	0.966	1.129
					331.6	1.119	0.966	1.129
					331.7	1.122	0.967	1.130
					331.9	1.122	0.967	1.130
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	332.1	1.124	0.968	1.131
					332.3	1.128	0.968	1.131
					332.5	1.129	0.969	1.132
					332.6	1.131	0.970	1.133
					332.8	1.132	0.970	1.133
					333.0	1.134	0.971	1.134
					333.2	1.136	0.971	1.134
					333.3	1.139	0.972	1.135
					333.5	1.140	0.972	1.135
					333.7	1.143	0.973	1.136
					333.9	1.144	0.973	1.136
					334.1	1.145	0.974	1.137

					334.2	1.145	0.974	1.137
					334.4	1.146	0.975	1.138
					334.6	1.145	0.976	1.139
					334.8	1.145	0.976	1.139
					334.9	1.148	0.977	1.140
					335.1	1.149	0.977	1.140
					335.3	1.151	0.978	1.141
					335.5	1.153	0.978	1.141
					335.7	1.156	0.979	1.142
					335.8	1.157	0.979	1.142
					336.0	1.158	0.980	1.143
					336.2	1.160	0.981	1.144
					336.4	1.161	0.981	1.144
					336.5	1.160	0.982	1.145
					336.7	1.162	0.982	1.145
					336.9	1.162	0.983	1.146
					337.1	1.162	0.983	1.146
					337.2	1.161	0.984	1.147

					337.4	1.159	0.984	1.147
					337.6	1.159	0.985	1.148
					337.8	1.160	0.985	1.149
					338.0	1.162	0.986	1.149
					338.1	1.163	0.987	1.150
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	338.3	1.163	0.987	1.150
					338.5	1.162	0.988	1.151
					338.7	1.164	0.988	1.151
					338.8	1.166	0.989	1.152
					339.0	1.168	0.989	1.152
					339.2	1.170	0.990	1.153
					339.4	1.173	0.990	1.153
					339.6	1.176	0.991	1.154
					339.7	1.181	0.992	1.155
					339.9	1.183	0.992	1.155
					340.1	1.186	0.993	1.156
					340.3	1.188	0.993	1.156
					340.4	1.191	0.994	1.157

					340.6	1.192	0.994	1.157
					340.8	1.194	0.995	1.158
					341.0	1.195	0.995	1.158
					341.1	1.196	0.996	1.159
					341.3	1.193	0.996	1.160
					341.5	1.193	0.997	1.160
					341.7	1.193	0.998	1.161
					341.9	1.194	0.998	1.161
					342.0	1.195	0.999	1.162
					342.2	1.197	0.999	1.162
					342.4	1.197	1.000	1.163
					342.6	1.199	1.000	1.163
					342.7	1.200	1.001	1.164
					342.9	1.198	1.001	1.164
					343.1	1.199	1.002	1.165
					343.3	1.197	1.003	1.166
					343.4	1.197	1.003	1.166
					343.6	1.200	1.004	1.167

					343.8	1.202	1.004	1.167
					344.0	1.204	1.005	1.168
					344.1	1.205	1.005	1.168
					344.3	1.205	1.006	1.169
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	344.5	1.206	1.006	1.169
					344.7	1.207	1.007	1.170
					344.9	1.209	1.008	1.171
					345.0	1.211	1.008	1.171
					345.2	1.212	1.009	1.172
					345.4	1.212	1.009	1.172
					345.6	1.210	1.010	1.173
					345.7	1.209	1.010	1.173
					345.9	1.207	1.011	1.174
					346.1	1.208	1.011	1.174
					346.3	1.205	1.012	1.175
					346.4	1.207	1.012	1.176
					346.6	1.208	1.013	1.176
					346.8	1.210	1.014	1.177

					347.0	1.213	1.014	1.177
					347.1	1.215	1.015	1.178
					347.3	1.214	1.015	1.178
					347.5	1.215	1.016	1.179
					347.7	1.215	1.016	1.179
					347.8	1.213	1.017	1.180
					348.0	1.214	1.017	1.180
					348.2	1.215	1.018	1.181
					348.4	1.218	1.019	1.182
					348.6	1.219	1.019	1.182
					348.7	1.220	1.020	1.183
					348.9	1.222	1.020	1.183
					349.1	1.223	1.021	1.184
					349.3	1.225	1.021	1.184
					349.4	1.227	1.022	1.185
					349.6	1.229	1.022	1.185
					349.8	1.232	1.023	1.186
					350.0	1.233	1.023	1.187

					350.1	1.235	1.024	1.187
					350.3	1.238	1.025	1.188
					350.5	1.239	1.025	1.188
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	350.7	1.238	1.026	1.189
					350.8	1.239	1.026	1.189
					351.0	1.238	1.027	1.190
					351.2	1.239	1.027	1.190
					351.4	1.238	1.028	1.191
					351.5	1.238	1.028	1.191
					351.7	1.237	1.029	1.192
					351.9	1.239	1.030	1.193
					352.1	1.239	1.030	1.193
					352.3	1.241	1.031	1.194
					352.4	1.241	1.031	1.194
					352.6	1.242	1.032	1.195
					352.8	1.244	1.032	1.195
					353.0	1.245	1.033	1.196
					353.1	1.245	1.033	1.196

					353.3	1.244	1.034	1.197
					353.5	1.244	1.035	1.198
					353.7	1.245	1.035	1.198
					353.8	1.245	1.036	1.199
					354.0	1.247	1.036	1.199
					354.2	1.248	1.037	1.200
					354.4	1.247	1.037	1.200
					354.5	1.248	1.038	1.201
					354.7	1.248	1.038	1.201
					354.9	1.249	1.039	1.202
					355.1	1.250	1.040	1.203
					355.2	1.250	1.040	1.203
					355.4	1.250	1.041	1.204
					355.6	1.250	1.041	1.204
					355.8	1.251	1.042	1.205
					355.9	1.252	1.042	1.205
					356.1	1.252	1.043	1.206
					356.3	1.255	1.043	1.206

					356.5	1.256	1.044	1.207
					356.7	1.257	1.045	1.208
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	356.8	1.259	1.045	1.208
					357.0	1.262	1.046	1.209
					357.2	1.265	1.046	1.209
					357.4	1.267	1.047	1.210
					357.5	1.268	1.047	1.210
					357.7	1.270	1.048	1.211
					357.9	1.272	1.048	1.211
					358.1	1.273	1.049	1.212
					358.2	1.275	1.050	1.213
					358.4	1.278	1.050	1.213
					358.6	1.279	1.051	1.214
					358.8	1.282	1.051	1.214
					358.9	1.284	1.052	1.215
					359.1	1.286	1.052	1.215
					359.3	1.286	1.053	1.216
					359.5	1.288	1.053	1.216

					359.6	1.290	1.054	1.217
					359.8	1.290	1.055	1.218
					360.0	1.291	1.055	1.218
					360.2	1.293	1.056	1.219
					360.3	1.296	1.056	1.219
					360.5	1.296	1.057	1.220
					360.7	1.297	1.057	1.220
					360.9	1.298	1.058	1.221
					361.0	1.298	1.058	1.221
					361.2	1.298	1.059	1.222
					361.4	1.298	1.060	1.223
					361.6	1.297	1.060	1.223
					361.7	1.297	1.061	1.224
					361.9	1.299	1.061	1.224
					362.1	1.303	1.062	1.225
					362.3	1.304	1.062	1.225
					362.4	1.307	1.063	1.226
					362.6	1.308	1.063	1.226

					362.8	1.312	1.064	1.227
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	363.0	1.313	1.065	1.228
					363.1	1.316	1.065	1.228
					363.3	1.318	1.066	1.229
					363.5	1.320	1.066	1.229
					363.7	1.323	1.067	1.230
					363.9	1.323	1.067	1.230
					364.0	1.323	1.068	1.231
					364.2	1.322	1.068	1.231
					364.4	1.323	1.069	1.232
					364.5	1.323	1.069	1.233
					364.7	1.323	1.070	1.233
					364.9	1.324	1.071	1.234
					365.1	1.323	1.071	1.234
					365.3	1.322	1.072	1.235
					365.4	1.323	1.072	1.235
					365.6	1.325	1.073	1.236
					365.8	1.326	1.073	1.236

					366.0	1.324	1.074	1.237
					366.1	1.324	1.075	1.238
					366.3	1.326	1.075	1.238
					366.5	1.326	1.076	1.239
					366.7	1.326	1.076	1.239
					366.8	1.327	1.077	1.240
					367.0	1.327	1.077	1.240
					367.2	1.329	1.078	1.241
					367.4	1.331	1.078	1.241
					367.5	1.332	1.079	1.242
					367.7	1.331	1.080	1.243
					367.9	1.330	1.080	1.243
					368.1	1.329	1.081	1.244
					368.2	1.330	1.081	1.244
					368.4	1.330	1.082	1.245
					368.6	1.330	1.082	1.245
					368.8	1.331	1.083	1.246
					368.9	1.330	1.083	1.246

Saccharine	C7H5NO3S	183.2	0.093	Test set 2	369.1	1.328	1.084	1.247
					369.3	1.330	1.085	1.248
					369.5	1.331	1.085	1.248
					369.6	1.334	1.086	1.249
					369.8	1.336	1.086	1.249
					370.0	1.337	1.087	1.250
					370.2	1.338	1.087	1.250
					370.3	1.339	1.088	1.251
					370.5	1.339	1.088	1.252
					370.7	1.340	1.089	1.252
					370.9	1.341	1.090	1.253
					371.0	1.342	1.090	1.253
					371.2	1.342	1.091	1.254
					371.4	1.344	1.091	1.254
					371.6	1.346	1.092	1.255
					371.7	1.347	1.092	1.255
					371.9	1.348	1.093	1.256
					372.1	1.348	1.093	1.257

					372.3	1.349	1.094	1.257
					372.4	1.349	1.095	1.258
					372.6	1.350	1.095	1.258
					372.8	1.350	1.096	1.259
					373.0	1.350	1.096	1.259
					373.1	1.350	1.097	1.260
					373.3	1.350	1.097	1.260
					373.5	1.350	1.098	1.261
					373.7	1.348	1.099	1.262
					373.8	1.347	1.099	1.262
					374.0	1.347	1.100	1.263
					374.2	1.347	1.100	1.263
					374.4	1.348	1.101	1.264
					374.5	1.352	1.101	1.264
					374.7	1.354	1.102	1.265
					374.9	1.356	1.102	1.265
					375.1	1.356	1.103	1.266
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	375.2	1.357	1.104	1.267

					375.4	1.356	1.104	1.267
					375.6	1.356	1.105	1.268
					375.8	1.355	1.105	1.268
					375.9	1.355	1.106	1.269
					376.1	1.357	1.106	1.269
					376.3	1.357	1.107	1.270
					376.5	1.360	1.107	1.271
					376.6	1.361	1.108	1.271
					376.8	1.363	1.109	1.272
					377.0	1.363	1.109	1.272
					377.2	1.362	1.110	1.273
					377.3	1.362	1.110	1.273
					377.5	1.363	1.111	1.274
					377.7	1.364	1.111	1.274
					377.9	1.365	1.112	1.275
					378.0	1.366	1.113	1.276
					378.2	1.365	1.113	1.276
					378.4	1.365	1.114	1.277

					378.6	1.367	1.114	1.277
					378.7	1.368	1.115	1.278
					378.9	1.367	1.115	1.278
					379.1	1.368	1.116	1.279
					379.3	1.367	1.116	1.279
					379.4	1.367	1.117	1.280
					379.6	1.367	1.118	1.281
					379.8	1.366	1.118	1.281
					380.0	1.366	1.119	1.282
					380.1	1.368	1.119	1.282
					380.3	1.370	1.120	1.283
					380.5	1.373	1.120	1.283
					380.7	1.374	1.121	1.284
					380.8	1.376	1.122	1.285
					381.0	1.378	1.122	1.285
					381.2	1.378	1.123	1.286
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	381.4	1.379	1.123	1.286
					381.5	1.381	1.124	1.287

					381.7	1.384	1.124	1.287
					381.9	1.388	1.125	1.288
					382.1	1.390	1.125	1.288
					382.2	1.390	1.126	1.289
					382.4	1.391	1.127	1.290
					382.6	1.391	1.127	1.290
					382.8	1.390	1.128	1.291
					382.9	1.391	1.128	1.291
					383.1	1.391	1.129	1.292
					383.3	1.391	1.129	1.292
					383.5	1.392	1.130	1.293
					383.6	1.390	1.131	1.294
					383.8	1.387	1.131	1.294
					384.0	1.385	1.132	1.295
					384.2	1.383	1.132	1.295
					384.3	1.382	1.133	1.296
					384.5	1.382	1.133	1.296
					384.7	1.380	1.134	1.297

					384.9	1.379	1.134	1.297
					385.0	1.380	1.135	1.298
					385.2	1.381	1.136	1.299
					385.4	1.380	1.136	1.299
					385.6	1.381	1.137	1.300
					385.7	1.379	1.137	1.300
					385.9	1.378	1.138	1.301
					386.1	1.376	1.138	1.301
					386.3	1.376	1.139	1.302
					386.4	1.376	1.140	1.303
					386.6	1.377	1.140	1.303
					386.8	1.381	1.141	1.304
					387.0	1.382	1.141	1.304
					387.1	1.383	1.142	1.305
					387.3	1.383	1.142	1.305
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	387.5	1.382	1.143	1.306
					387.7	1.381	1.144	1.307
					387.8	1.379	1.144	1.307

					388.0	1.380	1.145	1.308
					388.2	1.380	1.145	1.308
					388.4	1.380	1.146	1.309
					388.5	1.382	1.146	1.309
					388.7	1.382	1.147	1.310
					388.9	1.384	1.147	1.310
					389.1	1.383	1.148	1.311
					389.2	1.384	1.149	1.312
					389.4	1.385	1.149	1.312
					389.6	1.385	1.150	1.313
					389.8	1.386	1.150	1.313
					389.9	1.388	1.151	1.314
					390.1	1.388	1.151	1.314
					390.3	1.389	1.152	1.315
					390.5	1.389	1.153	1.316
					390.6	1.390	1.153	1.316
					390.8	1.391	1.154	1.317
					391.0	1.392	1.154	1.317

					391.2	1.394	1.155	1.318
					391.3	1.395	1.155	1.318
					391.5	1.396	1.156	1.319
					391.7	1.397	1.157	1.320
					391.9	1.396	1.157	1.320
					392.0	1.397	1.158	1.321
					392.2	1.397	1.158	1.321
					392.4	1.400	1.159	1.322
					392.6	1.402	1.159	1.322
					392.7	1.404	1.160	1.323
					392.9	1.405	1.160	1.323
					393.1	1.404	1.161	1.324
					393.3	1.404	1.162	1.325
					393.4	1.403	1.162	1.325
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	393.6	1.403	1.163	1.326
					393.8	1.403	1.163	1.326
					394.0	1.404	1.164	1.327
					394.1	1.405	1.164	1.327

					394.3	1.405	1.165	1.328
					394.5	1.407	1.166	1.329
					394.7	1.407	1.166	1.329
					394.8	1.408	1.167	1.330
					395.0	1.409	1.167	1.330
					395.2	1.411	1.168	1.331
					395.4	1.412	1.168	1.331
					395.5	1.412	1.169	1.332
					395.7	1.411	1.170	1.333
					395.9	1.412	1.170	1.333
					396.1	1.412	1.171	1.334
					396.2	1.413	1.171	1.334
					396.4	1.412	1.172	1.335
					396.6	1.412	1.172	1.335
					396.8	1.412	1.173	1.336
					396.9	1.412	1.174	1.337
					397.1	1.410	1.174	1.337
					397.3	1.411	1.175	1.338

					397.5	1.410	1.175	1.338
					397.6	1.411	1.176	1.339
					397.8	1.412	1.176	1.339
					398.0	1.409	1.177	1.340
					398.2	1.409	1.178	1.341
					398.3	1.408	1.178	1.341
					398.5	1.408	1.179	1.342
					398.7	1.410	1.179	1.342
					398.9	1.409	1.180	1.343
					399.0	1.409	1.180	1.343
					399.2	1.408	1.181	1.344
					399.4	1.409	1.181	1.345
					399.5	1.409	1.182	1.345
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	399.7	1.409	1.183	1.346
					399.9	1.408	1.183	1.346
					400.1	1.409	1.184	1.347
					400.2	1.408	1.184	1.347
					400.4	1.410	1.185	1.348

					400.6	1.410	1.185	1.349
					400.8	1.408	1.186	1.349
					400.9	1.410	1.187	1.350
					401.1	1.410	1.187	1.350
					401.3	1.411	1.188	1.351
					401.5	1.412	1.188	1.351
					401.6	1.412	1.189	1.352
					401.8	1.413	1.189	1.353
					402.0	1.415	1.190	1.353
					402.2	1.417	1.191	1.354
					402.3	1.418	1.191	1.354
					402.5	1.418	1.192	1.355
					402.7	1.421	1.192	1.355
					402.9	1.421	1.193	1.356
					403.0	1.422	1.193	1.357
					403.2	1.422	1.194	1.357
					403.4	1.423	1.195	1.358
					403.6	1.423	1.195	1.358

					403.7	1.423	1.196	1.359
					403.9	1.423	1.196	1.359
					404.1	1.425	1.197	1.360
					404.3	1.426	1.197	1.360
					404.4	1.426	1.198	1.361
					404.6	1.426	1.199	1.362
					404.8	1.426	1.199	1.362
					405.0	1.425	1.200	1.363
					405.1	1.427	1.200	1.363
					405.3	1.427	1.201	1.364
					405.5	1.430	1.201	1.364
					405.7	1.429	1.202	1.365
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	405.8	1.430	1.203	1.366
					406.0	1.430	1.203	1.366
					406.2	1.431	1.204	1.367
					406.4	1.431	1.204	1.367
					406.5	1.430	1.205	1.368
					406.7	1.430	1.205	1.369

					406.9	1.430	1.206	1.369
					407.1	1.432	1.207	1.370
					407.2	1.432	1.207	1.370
					407.4	1.433	1.208	1.371
					407.6	1.435	1.208	1.371
					407.8	1.435	1.209	1.372
					407.9	1.435	1.209	1.373
					408.1	1.436	1.210	1.373
					408.3	1.435	1.211	1.374
					408.5	1.435	1.211	1.374
					408.6	1.433	1.212	1.375
					408.8	1.434	1.212	1.375
					409.0	1.434	1.213	1.376
					409.2	1.435	1.213	1.377
					409.3	1.432	1.214	1.377
					409.5	1.431	1.215	1.378
					409.7	1.431	1.215	1.378
					409.9	1.432	1.216	1.379

					410.0	1.433	1.216	1.379
					410.2	1.433	1.217	1.380
					410.4	1.434	1.218	1.381
					410.6	1.436	1.218	1.381
					410.7	1.437	1.219	1.382
					410.9	1.438	1.219	1.382
					411.1	1.439	1.220	1.383
					411.3	1.440	1.220	1.383
					411.4	1.441	1.221	1.384
					411.6	1.443	1.222	1.385
					411.8	1.443	1.222	1.385
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	412.0	1.444	1.223	1.386
					412.1	1.447	1.223	1.386
					412.3	1.450	1.224	1.387
					412.5	1.454	1.224	1.387
					412.7	1.456	1.225	1.388
					412.8	1.457	1.226	1.389
					413.0	1.457	1.226	1.389

					413.2	1.457	1.227	1.390
					413.4	1.458	1.227	1.390
					413.5	1.460	1.228	1.391
					413.7	1.458	1.228	1.391
					413.9	1.457	1.229	1.392
					414.0	1.459	1.230	1.393
					414.2	1.460	1.230	1.393
					414.4	1.461	1.231	1.394
					414.6	1.462	1.231	1.394
					414.7	1.463	1.232	1.395
					414.9	1.464	1.232	1.396
					415.1	1.467	1.233	1.396
					415.3	1.470	1.234	1.397
					415.4	1.471	1.234	1.397
					415.6	1.472	1.235	1.398
					415.8	1.474	1.235	1.398
					416.0	1.476	1.236	1.399
					416.1	1.477	1.236	1.400

					416.3	1.479	1.237	1.400
					416.5	1.480	1.238	1.401
					416.7	1.479	1.238	1.401
					416.8	1.479	1.239	1.402
					417.0	1.480	1.239	1.402
					417.2	1.480	1.240	1.403
					417.4	1.478	1.241	1.404
					417.5	1.479	1.241	1.404
					417.7	1.480	1.242	1.405
					417.9	1.481	1.242	1.405
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	418.1	1.482	1.243	1.406
					418.2	1.483	1.243	1.406
					418.4	1.483	1.244	1.407
					418.6	1.484	1.245	1.408
					418.8	1.482	1.245	1.408
					418.9	1.481	1.246	1.409
					419.1	1.482	1.246	1.409
					419.3	1.483	1.247	1.410

					419.5	1.483	1.247	1.410
					419.6	1.485	1.248	1.411
					419.8	1.486	1.249	1.412
					420.0	1.486	1.249	1.412
					420.2	1.485	1.250	1.413
					420.3	1.484	1.250	1.413
					420.5	1.482	1.251	1.414
					420.7	1.481	1.252	1.415
					420.9	1.479	1.252	1.415
					421.0	1.477	1.253	1.416
					421.2	1.476	1.253	1.416
					421.4	1.475	1.254	1.417
					421.6	1.473	1.254	1.417
					421.7	1.474	1.255	1.418
					421.9	1.475	1.256	1.419
					422.1	1.476	1.256	1.419
					422.3	1.477	1.257	1.420
					422.4	1.479	1.257	1.420

					422.6	1.481	1.258	1.421
					422.8	1.483	1.258	1.421
					423.0	1.484	1.259	1.422
					423.1	1.485	1.260	1.423
					423.3	1.487	1.260	1.423
					423.5	1.490	1.261	1.424
					423.7	1.492	1.261	1.424
					423.8	1.495	1.262	1.425
					424.0	1.495	1.263	1.426
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	424.2	1.497	1.263	1.426
					424.4	1.499	1.264	1.427
					424.5	1.498	1.264	1.427
					424.7	1.496	1.265	1.428
					424.9	1.496	1.265	1.428
					425.1	1.497	1.266	1.429
					425.2	1.499	1.267	1.430
					425.4	1.502	1.267	1.430
					425.6	1.506	1.268	1.431

					425.8	1.506	1.268	1.431
					425.9	1.510	1.269	1.432
					426.1	1.511	1.269	1.433
					426.3	1.512	1.270	1.433
					426.4	1.514	1.271	1.434
					426.6	1.514	1.271	1.434
					426.8	1.515	1.272	1.435
					427.0	1.515	1.272	1.435
					427.1	1.518	1.273	1.436
					427.3	1.519	1.274	1.437
					427.5	1.524	1.274	1.437
					427.7	1.527	1.275	1.438
					427.8	1.529	1.275	1.438
					428.0	1.530	1.276	1.439
					428.2	1.531	1.276	1.439
					428.4	1.534	1.277	1.440
					428.5	1.537	1.278	1.441
					428.7	1.538	1.278	1.441

					428.9	1.537	1.279	1.442
					429.1	1.538	1.279	1.442
					429.2	1.538	1.280	1.443
					429.4	1.538	1.281	1.444
					429.6	1.538	1.281	1.444
					429.8	1.538	1.282	1.445
					429.9	1.536	1.282	1.445
					430.1	1.535	1.283	1.446
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	430.3	1.532	1.283	1.446
					430.5	1.531	1.284	1.447
					430.6	1.531	1.285	1.448
					430.8	1.533	1.285	1.448
					431.0	1.534	1.286	1.449
					431.2	1.535	1.286	1.449
					431.3	1.537	1.287	1.450
					431.5	1.538	1.288	1.451
					431.7	1.541	1.288	1.451
					431.9	1.541	1.289	1.452

					432.0	1.541	1.289	1.452
					432.2	1.542	1.290	1.453
					432.4	1.542	1.290	1.453
					432.6	1.542	1.291	1.454
					432.7	1.541	1.292	1.455
					432.9	1.540	1.292	1.455
					433.1	1.538	1.293	1.456
					433.3	1.539	1.293	1.456
					433.4	1.537	1.294	1.457
					433.6	1.539	1.295	1.458
					433.8	1.543	1.295	1.458
					434.0	1.549	1.296	1.459
					434.1	1.551	1.296	1.459
					434.3	1.552	1.297	1.460
					434.5	1.552	1.297	1.460
					434.7	1.554	1.298	1.461
					434.8	1.554	1.299	1.462
					435.0	1.555	1.299	1.462

					435.2	1.555	1.300	1.463
					435.4	1.553	1.300	1.463
					435.5	1.555	1.301	1.464
					435.7	1.559	1.302	1.465
					435.9	1.562	1.302	1.465
					436.1	1.560	1.303	1.466
					436.2	1.558	1.303	1.466
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	436.4	1.558	1.304	1.467
					436.6	1.559	1.304	1.467
					436.8	1.561	1.305	1.468
					436.9	1.563	1.306	1.469
					437.1	1.563	1.306	1.469
					437.3	1.561	1.307	1.470
					437.4	1.562	1.307	1.470
					437.6	1.564	1.308	1.471
					437.8	1.565	1.309	1.472
					438.0	1.565	1.309	1.472
					438.1	1.567	1.310	1.473

					438.3	1.568	1.310	1.473
					438.5	1.569	1.311	1.474
					438.7	1.571	1.311	1.475
					438.8	1.571	1.312	1.475
					439.0	1.572	1.313	1.476
					439.2	1.572	1.313	1.476
					439.4	1.572	1.314	1.477
					439.5	1.571	1.314	1.477
					439.7	1.569	1.315	1.478
					439.9	1.568	1.316	1.479
					440.1	1.566	1.316	1.479
					440.2	1.566	1.317	1.480
					440.4	1.567	1.317	1.480
					440.6	1.567	1.318	1.481
					440.8	1.569	1.319	1.482
					440.9	1.571	1.319	1.482
					441.1	1.571	1.320	1.483
					441.3	1.572	1.320	1.483

					441.5	1.574	1.321	1.484
					441.6	1.574	1.321	1.485
					441.8	1.575	1.322	1.485
					442.0	1.576	1.323	1.486
					442.2	1.577	1.323	1.486
					442.3	1.577	1.324	1.487
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	442.5	1.579	1.324	1.487
					442.7	1.579	1.325	1.488
					442.9	1.581	1.326	1.489
					443.0	1.583	1.326	1.489
					443.2	1.585	1.327	1.490
					443.4	1.585	1.327	1.490
					443.6	1.585	1.328	1.491
					443.7	1.584	1.329	1.492
					443.9	1.584	1.329	1.492
					444.1	1.584	1.330	1.493
					444.3	1.583	1.330	1.493
					444.4	1.584	1.331	1.494

					444.6	1.585	1.331	1.494
					444.8	1.584	1.332	1.495
					445.0	1.586	1.333	1.496
					445.1	1.589	1.333	1.496
					445.3	1.590	1.334	1.497
					445.5	1.590	1.334	1.497
					445.7	1.591	1.335	1.498
					445.8	1.591	1.336	1.499
					446.0	1.592	1.336	1.499
					446.2	1.593	1.337	1.500
					446.4	1.595	1.337	1.500
					446.5	1.595	1.338	1.501
					446.7	1.595	1.339	1.502
					446.9	1.595	1.339	1.502
					447.1	1.595	1.340	1.503
					447.2	1.595	1.340	1.503
					447.4	1.594	1.341	1.504
					447.6	1.594	1.341	1.504

					447.8	1.594	1.342	1.505
					447.9	1.594	1.343	1.506
					448.1	1.593	1.343	1.506
					448.3	1.592	1.344	1.507
					448.4	1.592	1.344	1.507
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	448.6	1.593	1.345	1.508
					448.8	1.597	1.346	1.509
					449.0	1.600	1.346	1.509
					449.1	1.603	1.347	1.510
					449.3	1.605	1.347	1.510
					449.5	1.606	1.348	1.511
					449.7	1.606	1.349	1.512
					449.8	1.607	1.349	1.512
					450.0	1.605	1.350	1.513
					450.2	1.604	1.350	1.513
					450.4	1.603	1.351	1.514
					450.5	1.602	1.352	1.515
					450.7	1.602	1.352	1.515

					450.9	1.604	1.353	1.516
					451.1	1.604	1.353	1.516
					451.2	1.606	1.354	1.517
					451.4	1.607	1.354	1.517
					451.6	1.611	1.355	1.518
					451.8	1.613	1.356	1.519
					451.9	1.612	1.356	1.519
					452.1	1.614	1.357	1.520
					452.3	1.615	1.357	1.520
					452.5	1.615	1.358	1.521
					452.6	1.615	1.359	1.522
					452.8	1.614	1.359	1.522
					453.0	1.614	1.360	1.523
					453.2	1.617	1.360	1.523
					453.3	1.619	1.361	1.524
					453.5	1.622	1.362	1.525
					453.7	1.623	1.362	1.525
					453.9	1.623	1.363	1.526

					454.0	1.622	1.363	1.526
					454.2	1.622	1.364	1.527
					454.4	1.622	1.365	1.528
					454.6	1.624	1.365	1.528
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	454.7	1.627	1.366	1.529
					454.9	1.629	1.366	1.529
					455.1	1.630	1.367	1.530
					455.3	1.632	1.367	1.531
					455.4	1.632	1.368	1.531
					455.6	1.634	1.369	1.532
					455.8	1.635	1.369	1.532
					456.0	1.636	1.370	1.533
					456.1	1.637	1.370	1.534
					456.3	1.639	1.371	1.534
					456.5	1.642	1.372	1.535
					456.7	1.641	1.372	1.535
					456.8	1.642	1.373	1.536
					457.0	1.642	1.373	1.536

					457.2	1.642	1.374	1.537
					457.4	1.644	1.375	1.538
					457.5	1.645	1.375	1.538
					457.7	1.644	1.376	1.539
					457.9	1.644	1.376	1.539
					458.1	1.643	1.377	1.540
					458.2	1.644	1.378	1.541
					458.4	1.646	1.378	1.541
					458.6	1.647	1.379	1.542
					458.7	1.648	1.379	1.542
					458.9	1.649	1.380	1.543
					459.1	1.651	1.381	1.544
					459.3	1.653	1.381	1.544
					459.4	1.654	1.382	1.545
					459.6	1.653	1.382	1.545
					459.8	1.654	1.383	1.546
					460.0	1.653	1.384	1.547
					460.1	1.654	1.384	1.547

					460.3	1.654	1.385	1.548
					460.5	1.654	1.385	1.548
					460.7	1.654	1.386	1.549
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	460.8	1.654	1.387	1.550
					461.0	1.653	1.387	1.550
					461.2	1.652	1.388	1.551
					461.4	1.651	1.388	1.551
					461.5	1.650	1.389	1.552
					461.7	1.651	1.389	1.553
					461.9	1.652	1.390	1.553
					462.1	1.653	1.391	1.554
					462.2	1.653	1.391	1.554
					462.4	1.654	1.392	1.555
					462.6	1.654	1.392	1.556
					462.8	1.655	1.393	1.556
					462.9	1.658	1.394	1.557
					463.1	1.661	1.394	1.557
					463.3	1.663	1.395	1.558

					463.5	1.665	1.395	1.559
					463.6	1.665	1.396	1.559
					463.8	1.667	1.397	1.560
					464.0	1.667	1.397	1.560
					464.2	1.669	1.398	1.561
					464.3	1.671	1.398	1.561
					464.5	1.671	1.399	1.562
					464.7	1.670	1.400	1.563
					464.9	1.670	1.400	1.563
					465.0	1.669	1.401	1.564
					465.2	1.668	1.401	1.564
					465.4	1.668	1.402	1.565
					465.6	1.671	1.403	1.566
					465.7	1.674	1.403	1.566
					465.9	1.674	1.404	1.567
					466.1	1.675	1.404	1.567
					466.3	1.676	1.405	1.568
					466.4	1.678	1.406	1.569

					466.6	1.677	1.406	1.569
					466.8	1.678	1.407	1.570
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	467.0	1.681	1.407	1.570
					467.1	1.682	1.408	1.571
					467.3	1.683	1.409	1.572
					467.5	1.684	1.409	1.572
					467.7	1.684	1.410	1.573
					467.8	1.685	1.410	1.573
					468.0	1.684	1.411	1.574
					468.2	1.685	1.412	1.575
					468.4	1.688	1.412	1.575
					468.5	1.688	1.413	1.576
					468.7	1.685	1.413	1.576
					468.9	1.684	1.414	1.577
					469.1	1.682	1.415	1.578
					469.2	1.683	1.415	1.578
					469.4	1.682	1.416	1.579
					469.6	1.680	1.416	1.579

					469.7	1.681	1.417	1.580
					469.9	1.683	1.418	1.581
					470.1	1.683	1.418	1.581
					470.3	1.684	1.419	1.582
					470.4	1.684	1.419	1.582
					470.6	1.682	1.420	1.583
					470.8	1.680	1.421	1.584
					471.0	1.680	1.421	1.584
					471.1	1.679	1.422	1.585
					471.3	1.678	1.422	1.585
					471.5	1.678	1.423	1.586
					471.7	1.676	1.424	1.587
					471.8	1.674	1.424	1.587
					472.0	1.672	1.425	1.588
					472.2	1.667	1.425	1.588
					472.4	1.646	1.426	1.589
					472.5	1.638	1.427	1.590
					472.7	1.636	1.427	1.590

					472.9	1.635	1.428	1.591
Saccharine	C7H5NO3S	183.2	0.093	Test set 2	473.1	1.638	1.428	1.591
					473.2	1.640	1.429	1.592
					473.4	1.643	1.430	1.593
					473.6	1.645	1.430	1.593
					473.8	1.648	1.431	1.594
					473.9	1.650	1.431	1.594
					474.1	1.650	1.432	1.595
					474.3	1.650	1.433	1.596
					474.5	1.648	1.433	1.596
					474.6	1.649	1.434	1.597
					474.8	1.650	1.434	1.597
					475.0	1.650	1.435	1.598
					475.2	1.652	1.436	1.599
					475.3	1.653	1.436	1.599
					475.5	1.654	1.437	1.600
					475.7	1.657	1.437	1.600
					475.9	1.660	1.438	1.601

					476.0	1.665	1.439	1.602
					476.2	1.669	1.439	1.602
					476.4	1.671	1.440	1.603
					476.6	1.673	1.440	1.603
					476.7	1.675	1.441	1.604
					476.9	1.676	1.442	1.605
					477.1	1.678	1.442	1.605
					477.3	1.678	1.443	1.606
					477.4	1.679	1.443	1.606
					477.6	1.680	1.444	1.607
					477.8	1.680	1.445	1.608
					477.9	1.680	1.445	1.608
					478.1	1.680	1.446	1.609
					478.3	1.685	1.446	1.609
					478.5	1.688	1.447	1.610
					478.6	1.693	1.448	1.611
					478.8	1.695	1.448	1.611
					479.0	1.696	1.449	1.612

Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	479.2	1.695	1.449	1.613
					479.3	1.695	1.450	1.613
					479.5	1.697	1.451	1.614
					479.7	1.699	1.451	1.614
					479.9	1.703	1.452	1.615
					480.0	1.708	1.452	1.616
					480.2	1.714	1.453	1.616
					356.3	1.372	1.283	1.468
					356.5	1.376	1.284	1.468
					356.6	1.378	1.284	1.469
					356.8	1.380	1.285	1.470
					357.0	1.382	1.286	1.470
					357.2	1.383	1.286	1.471
					357.3	1.384	1.287	1.472
					357.5	1.386	1.288	1.472
					357.7	1.386	1.288	1.473
					357.9	1.389	1.289	1.474
					358.0	1.390	1.289	1.474

					358.2	1.391	1.290	1.475
					358.4	1.393	1.291	1.475
					358.6	1.395	1.291	1.476
					358.8	1.398	1.292	1.477
					358.9	1.400	1.293	1.477
					359.1	1.403	1.293	1.478
					359.3	1.406	1.294	1.479
					359.5	1.409	1.295	1.479
					359.6	1.411	1.295	1.480
					359.8	1.413	1.296	1.481
					360.0	1.415	1.297	1.481
					360.2	1.417	1.297	1.482
					360.3	1.417	1.298	1.483
					360.5	1.417	1.299	1.483
					360.7	1.419	1.299	1.484
					360.9	1.421	1.300	1.485
					361.0	1.423	1.301	1.485
Sodium	C6H12NNaO3S	201.2	0.119	Test set 2	361.2	1.425	1.301	1.486

Cyclamate					361.4	1.427	1.302	1.487
					361.6	1.428	1.302	1.487
					361.7	1.430	1.303	1.488
					361.9	1.431	1.304	1.488
					362.1	1.432	1.304	1.489
					362.3	1.433	1.305	1.490
					362.4	1.434	1.306	1.490
					362.6	1.435	1.306	1.491
					362.8	1.437	1.307	1.492
					363.0	1.438	1.308	1.492
					363.1	1.440	1.308	1.493
					363.3	1.441	1.309	1.494
					363.5	1.443	1.310	1.494
					363.7	1.445	1.310	1.495
					363.8	1.447	1.311	1.496
					364.0	1.448	1.312	1.496
					364.2	1.449	1.312	1.497
					364.4	1.450	1.313	1.498

					364.5	1.450	1.314	1.498
					364.7	1.450	1.314	1.499
					364.9	1.451	1.315	1.500
					365.1	1.452	1.315	1.500
					365.2	1.454	1.316	1.501
					365.4	1.456	1.317	1.502
					365.6	1.458	1.317	1.502
					365.8	1.458	1.318	1.503
					365.9	1.460	1.319	1.503
					366.1	1.462	1.319	1.504
					366.3	1.462	1.320	1.505
					366.5	1.462	1.321	1.505
					366.6	1.462	1.321	1.506
					366.8	1.462	1.322	1.507
					367.0	1.463	1.323	1.507
					367.2	1.465	1.323	1.508
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	367.3	1.466	1.324	1.509
					367.5	1.467	1.325	1.509

					367.7	1.467	1.325	1.510
					367.9	1.468	1.326	1.511
					368.1	1.468	1.327	1.511
					368.2	1.469	1.327	1.512
					368.4	1.468	1.328	1.513
					368.6	1.470	1.329	1.513
					368.8	1.472	1.329	1.514
					368.9	1.473	1.330	1.515
					369.1	1.475	1.331	1.515
					369.3	1.477	1.331	1.516
					369.5	1.478	1.332	1.517
					369.6	1.478	1.332	1.517
					369.8	1.478	1.333	1.518
					370.0	1.479	1.334	1.518
					370.2	1.480	1.334	1.519
					370.3	1.480	1.335	1.520
					370.5	1.480	1.336	1.520
					370.7	1.481	1.336	1.521

					370.9	1.480	1.337	1.522
					371.0	1.479	1.338	1.522
					371.2	1.478	1.338	1.523
					371.4	1.478	1.339	1.524
					371.6	1.479	1.340	1.524
					371.7	1.481	1.340	1.525
					371.9	1.482	1.341	1.526
					372.1	1.483	1.342	1.526
					372.3	1.485	1.342	1.527
					372.4	1.487	1.343	1.528
					372.6	1.488	1.344	1.528
					372.8	1.489	1.344	1.529
					373.0	1.490	1.345	1.530
					373.1	1.491	1.346	1.530
					373.3	1.491	1.346	1.531
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	373.5	1.492	1.347	1.532
					373.7	1.492	1.347	1.532
					373.8	1.493	1.348	1.533

					374.0	1.493	1.349	1.534
					374.2	1.493	1.349	1.534
					374.4	1.494	1.350	1.535
					374.5	1.494	1.351	1.536
					374.7	1.495	1.351	1.536
					374.9	1.496	1.352	1.537
					375.1	1.497	1.353	1.537
					375.2	1.498	1.353	1.538
					375.4	1.499	1.354	1.539
					375.6	1.499	1.355	1.539
					375.8	1.499	1.355	1.540
					375.9	1.500	1.356	1.541
					376.1	1.501	1.357	1.541
					376.3	1.502	1.357	1.542
					376.5	1.505	1.358	1.543
					376.6	1.508	1.359	1.543
					376.8	1.509	1.359	1.544
					377.0	1.509	1.360	1.545

					377.2	1.509	1.361	1.545
					377.3	1.510	1.361	1.546
					377.5	1.511	1.362	1.547
					377.7	1.513	1.363	1.547
					377.9	1.515	1.363	1.548
					378.0	1.516	1.364	1.549
					378.2	1.519	1.365	1.549
					378.4	1.522	1.365	1.550
					378.6	1.525	1.366	1.551
					378.7	1.527	1.367	1.551
					378.9	1.528	1.367	1.552
					379.1	1.529	1.368	1.553
					379.3	1.530	1.369	1.553
					379.4	1.531	1.369	1.554
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	379.6	1.531	1.370	1.555
					379.8	1.532	1.370	1.555
					380.0	1.533	1.371	1.556
					380.1	1.534	1.372	1.557

					380.3	1.535	1.372	1.557
					380.5	1.535	1.373	1.558
					380.7	1.536	1.374	1.558
					380.8	1.537	1.374	1.559
					381.0	1.538	1.375	1.560
					381.2	1.538	1.376	1.560
					381.4	1.538	1.376	1.561
					381.5	1.539	1.377	1.562
					381.7	1.539	1.378	1.562
					381.9	1.539	1.378	1.563
					382.1	1.539	1.379	1.564
					382.2	1.541	1.380	1.564
					382.4	1.542	1.380	1.565
					382.6	1.544	1.381	1.566
					382.8	1.545	1.382	1.566
					382.9	1.547	1.382	1.567
					383.1	1.548	1.383	1.568
					383.3	1.550	1.384	1.568

					383.5	1.550	1.384	1.569
					383.6	1.550	1.385	1.570
					383.8	1.550	1.386	1.570
					384.0	1.550	1.386	1.571
					384.2	1.550	1.387	1.572
					384.3	1.551	1.388	1.572
					384.5	1.551	1.388	1.573
					384.7	1.551	1.389	1.574
					384.9	1.550	1.390	1.574
					385.0	1.550	1.390	1.575
					385.2	1.550	1.391	1.576
					385.4	1.549	1.392	1.576
					385.6	1.548	1.392	1.577
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	385.7	1.547	1.393	1.578
					385.9	1.547	1.393	1.578
					386.1	1.546	1.394	1.579
					386.3	1.545	1.395	1.580
					386.4	1.545	1.395	1.580

					386.6	1.545	1.396	1.581
					386.8	1.546	1.397	1.582
					387.0	1.547	1.397	1.582
					387.1	1.548	1.398	1.583
					387.3	1.549	1.399	1.583
					387.5	1.549	1.399	1.584
					387.7	1.549	1.400	1.585
					387.8	1.549	1.401	1.585
					388.0	1.549	1.401	1.586
					388.2	1.550	1.402	1.587
					388.4	1.551	1.403	1.587
					388.5	1.551	1.403	1.588
					388.7	1.551	1.404	1.589
					388.9	1.551	1.405	1.589
					389.1	1.551	1.405	1.590
					389.2	1.551	1.406	1.591
					389.4	1.551	1.407	1.591
					389.6	1.552	1.407	1.592

					389.8	1.553	1.408	1.593
					389.9	1.554	1.409	1.593
					390.1	1.556	1.409	1.594
					390.3	1.560	1.410	1.595
					390.5	1.562	1.411	1.595
					390.6	1.564	1.411	1.596
					390.8	1.566	1.412	1.597
					391.0	1.567	1.413	1.597
					391.2	1.567	1.413	1.598
					391.3	1.567	1.414	1.599
					391.5	1.567	1.415	1.599
					391.7	1.567	1.415	1.600
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	391.9	1.567	1.416	1.601
					392.0	1.566	1.417	1.601
					392.2	1.565	1.417	1.602
					392.4	1.566	1.418	1.603
					392.6	1.568	1.419	1.603
					392.7	1.569	1.419	1.604

					392.9	1.570	1.420	1.605
					393.1	1.570	1.421	1.605
					393.3	1.571	1.421	1.606
					393.4	1.571	1.422	1.607
					393.6	1.572	1.423	1.607
					393.8	1.572	1.423	1.608
					394.0	1.573	1.424	1.609
					394.1	1.573	1.425	1.609
					394.3	1.572	1.425	1.610
					394.5	1.573	1.426	1.611
					394.7	1.574	1.427	1.611
					394.8	1.576	1.427	1.612
					395.0	1.577	1.428	1.613
					395.2	1.578	1.429	1.613
					395.4	1.578	1.429	1.614
					395.5	1.579	1.430	1.615
					395.7	1.580	1.431	1.615
					395.9	1.579	1.431	1.616

					396.1	1.579	1.432	1.617
					396.2	1.581	1.432	1.617
					396.4	1.582	1.433	1.618
					396.6	1.581	1.434	1.619
					396.8	1.581	1.435	1.619
					396.9	1.582	1.435	1.620
					397.1	1.583	1.436	1.621
					397.3	1.584	1.436	1.621
					397.5	1.585	1.437	1.622
					397.6	1.586	1.438	1.623
					397.8	1.586	1.438	1.623
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	398.0	1.586	1.439	1.624
					398.1	1.586	1.440	1.625
					398.3	1.585	1.440	1.625
					398.5	1.584	1.441	1.626
					398.7	1.584	1.442	1.627
					398.8	1.584	1.442	1.627
					399.0	1.583	1.443	1.628

					399.2	1.584	1.444	1.628
					399.4	1.585	1.444	1.629
					399.5	1.586	1.445	1.630
					399.7	1.586	1.446	1.631
					399.9	1.586	1.446	1.631
					400.1	1.586	1.447	1.632
					400.2	1.586	1.448	1.632
					400.4	1.586	1.448	1.633
					400.6	1.586	1.449	1.634
					400.8	1.586	1.450	1.635
					400.9	1.586	1.450	1.635
					401.1	1.586	1.451	1.636
					401.3	1.587	1.452	1.636
					401.5	1.587	1.452	1.637
					401.6	1.587	1.453	1.638
					401.8	1.587	1.454	1.638
					402.0	1.587	1.454	1.639
					402.2	1.587	1.455	1.640

					402.3	1.587	1.456	1.640
					402.5	1.587	1.456	1.641
					402.7	1.587	1.457	1.642
					402.9	1.587	1.458	1.642
					403.0	1.588	1.458	1.643
					403.2	1.587	1.459	1.644
					403.4	1.588	1.460	1.644
					403.6	1.588	1.460	1.645
					403.7	1.588	1.461	1.646
					403.9	1.589	1.462	1.646
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	404.1	1.591	1.462	1.647
					404.3	1.593	1.463	1.648
					404.4	1.593	1.464	1.648
					404.6	1.594	1.464	1.649
					404.8	1.595	1.465	1.650
					405.0	1.595	1.466	1.650
					405.1	1.595	1.466	1.651
					405.3	1.595	1.467	1.652

					405.5	1.595	1.468	1.652
					405.7	1.595	1.468	1.653
					405.8	1.595	1.469	1.654
					406.0	1.596	1.470	1.654
					406.2	1.597	1.470	1.655
					406.4	1.598	1.471	1.656
					406.5	1.599	1.472	1.656
					406.7	1.599	1.472	1.657
					406.9	1.601	1.473	1.658
					407.1	1.603	1.474	1.658
					407.2	1.605	1.474	1.659
					407.4	1.605	1.475	1.660
					407.6	1.605	1.476	1.660
					407.8	1.607	1.476	1.661
					407.9	1.608	1.477	1.662
					408.1	1.609	1.478	1.662
					408.3	1.609	1.478	1.663
					408.5	1.609	1.479	1.664

					408.6	1.608	1.480	1.664
					408.8	1.608	1.480	1.665
					409.0	1.610	1.481	1.666
					409.2	1.613	1.482	1.666
					409.3	1.615	1.482	1.667
					409.5	1.616	1.483	1.668
					409.7	1.616	1.484	1.668
					409.9	1.617	1.484	1.669
					410.0	1.618	1.485	1.670
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	410.2	1.620	1.486	1.670
					410.4	1.622	1.486	1.671
					410.6	1.622	1.487	1.672
					410.7	1.623	1.488	1.673
					410.9	1.623	1.488	1.673
					411.1	1.624	1.489	1.674
					411.3	1.625	1.490	1.675
					411.4	1.624	1.490	1.675
					411.6	1.624	1.491	1.676

					411.8	1.625	1.492	1.676
					412.0	1.625	1.492	1.677
					412.1	1.625	1.493	1.678
					412.3	1.626	1.494	1.679
					412.5	1.626	1.494	1.679
					412.7	1.626	1.495	1.680
					412.8	1.627	1.496	1.681
					413.0	1.628	1.496	1.681
					413.2	1.629	1.497	1.682
					413.4	1.629	1.498	1.683
					413.5	1.630	1.498	1.683
					413.7	1.630	1.499	1.684
					413.9	1.631	1.500	1.685
					414.1	1.631	1.501	1.685
					414.2	1.632	1.501	1.686
					414.4	1.632	1.502	1.687
					414.6	1.633	1.503	1.687
					414.7	1.634	1.503	1.688

					414.9	1.634	1.504	1.689
					415.1	1.634	1.504	1.689
					415.3	1.635	1.505	1.690
					415.4	1.636	1.506	1.691
					415.6	1.637	1.507	1.691
					415.8	1.639	1.507	1.692
					416.0	1.640	1.508	1.693
					416.1	1.646	1.509	1.693
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	416.3	1.645	1.509	1.694
					416.5	1.639	1.510	1.695
					416.7	1.633	1.511	1.695
					416.8	1.630	1.511	1.696
					417.0	1.631	1.512	1.697
					417.2	1.633	1.513	1.697
					417.4	1.635	1.513	1.698
					417.5	1.637	1.514	1.699
					417.7	1.637	1.515	1.699
					417.9	1.637	1.515	1.700

					418.1	1.638	1.516	1.701
					418.2	1.639	1.517	1.701
					418.4	1.641	1.517	1.702
					418.6	1.643	1.518	1.703
					418.8	1.644	1.519	1.703
					418.9	1.645	1.519	1.704
					419.1	1.647	1.520	1.705
					419.3	1.648	1.521	1.705
					419.5	1.650	1.521	1.706
					419.6	1.650	1.522	1.707
					419.8	1.650	1.523	1.707
					420.0	1.650	1.523	1.708
					420.2	1.651	1.524	1.709
					420.3	1.653	1.525	1.709
					420.5	1.655	1.525	1.710
					420.7	1.656	1.526	1.711
					420.9	1.657	1.527	1.711
					421.0	1.658	1.527	1.712

					421.2	1.659	1.528	1.713
					421.4	1.661	1.529	1.713
					421.6	1.663	1.529	1.714
					421.7	1.665	1.530	1.715
					421.9	1.668	1.531	1.715
					422.1	1.669	1.531	1.716
					422.3	1.669	1.532	1.717
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	422.4	1.669	1.533	1.717
					422.6	1.669	1.533	1.718
					422.8	1.669	1.534	1.719
					423.0	1.669	1.535	1.719
					423.1	1.669	1.535	1.720
					423.3	1.670	1.536	1.721
					423.5	1.671	1.537	1.722
					423.7	1.671	1.537	1.722
					423.8	1.671	1.538	1.723
					424.0	1.672	1.539	1.724
					424.2	1.674	1.539	1.724

					424.4	1.675	1.540	1.725
					424.5	1.675	1.541	1.726
					424.7	1.675	1.541	1.726
					424.9	1.676	1.542	1.727
					425.1	1.677	1.543	1.728
					425.2	1.678	1.544	1.728
					425.4	1.679	1.544	1.729
					425.6	1.680	1.545	1.730
					425.8	1.679	1.546	1.730
					425.9	1.679	1.546	1.731
					426.1	1.680	1.547	1.732
					426.3	1.680	1.548	1.732
					426.5	1.680	1.548	1.733
					426.6	1.680	1.549	1.734
					426.8	1.681	1.550	1.734
					427.0	1.681	1.550	1.735
					427.2	1.681	1.551	1.736
					427.3	1.681	1.552	1.736

					427.5	1.681	1.552	1.737
					427.7	1.682	1.553	1.738
					427.9	1.682	1.554	1.738
					428.0	1.681	1.554	1.739
					428.2	1.680	1.555	1.740
					428.4	1.678	1.556	1.740
Sodium Cyclamate	C6H12NNaO3S	201.2	0.119	Test set 2	428.5	1.676	1.556	1.741
					428.7	1.676	1.557	1.742
					428.9	1.675	1.558	1.742
					429.1	1.675	1.558	1.743
					429.2	1.676	1.559	1.744
					429.4	1.676	1.560	1.744
					429.6	1.676	1.560	1.745
					429.8	1.676	1.561	1.746
					429.9	1.676	1.562	1.746
					430.1	1.677	1.562	1.747
					430.3	1.678	1.563	1.748
					430.5	1.679	1.564	1.749

					430.6	1.679	1.564	1.749
					430.8	1.679	1.565	1.750
					431.0	1.678	1.566	1.751
					431.2	1.678	1.566	1.751
					431.3	1.679	1.567	1.752
					431.5	1.678	1.568	1.753
					431.7	1.679	1.569	1.753
					431.9	1.679	1.569	1.754
					432.0	1.679	1.570	1.755
					432.2	1.679	1.571	1.755
					432.4	1.678	1.571	1.756
					432.6	1.677	1.572	1.757
					432.7	1.677	1.573	1.757
					432.9	1.676	1.573	1.758
					433.1	1.675	1.574	1.759
					433.3	1.674	1.575	1.759
					433.4	1.673	1.575	1.760
					433.6	1.672	1.576	1.761

					433.8	1.672	1.577	1.761
					434.0	1.673	1.577	1.762
					434.1	1.674	1.578	1.763
					434.3	1.673	1.579	1.763
					434.5	1.673	1.579	1.764
Aspartame	C14H18N2O	294.3	0.132	Test set 2	434.7	1.673	1.580	1.765
					434.8	1.673	1.581	1.765
					435.0	1.673	1.581	1.766
					435.2	1.672	1.582	1.767
					435.4	1.671	1.583	1.768
					435.5	1.672	1.583	1.768
					435.7	1.673	1.584	1.769
					435.9	1.673	1.585	1.770
					436.1	1.673	1.585	1.770
					436.2	1.672	1.586	1.771
					436.4	1.671	1.587	1.772
					335.1	1.283	1.311	1.427
					335.3	1.283	1.311	1.428

					335.5	1.282	1.312	1.429
					335.6	1.280	1.313	1.429
					335.8	1.280	1.314	1.430
					336.0	1.281	1.314	1.431
					336.2	1.282	1.315	1.432
					336.3	1.282	1.316	1.432
					336.5	1.285	1.316	1.433
					336.7	1.288	1.317	1.434
					336.9	1.290	1.318	1.434
					337.1	1.292	1.318	1.435
					337.2	1.292	1.319	1.436
					337.4	1.291	1.320	1.436
					337.6	1.290	1.320	1.437
					337.8	1.293	1.321	1.438
					337.9	1.296	1.322	1.438
					338.1	1.297	1.322	1.439
					338.3	1.299	1.323	1.440
					338.5	1.301	1.324	1.440

					338.6	1.303	1.325	1.441
					338.8	1.305	1.325	1.442
					339.0	1.307	1.326	1.443
					339.2	1.310	1.327	1.443
Aspartame	C14H18N2O	294.3	0.132	Test set 2	339.4	1.311	1.327	1.444
					339.5	1.313	1.328	1.445
					339.7	1.315	1.329	1.445
					339.9	1.316	1.329	1.446
					340.1	1.317	1.330	1.447
					340.2	1.318	1.331	1.447
					340.4	1.321	1.331	1.448
					340.6	1.323	1.332	1.449
					340.8	1.325	1.333	1.449
					340.9	1.328	1.333	1.450
					341.1	1.332	1.334	1.451
					341.3	1.337	1.335	1.451
					341.5	1.341	1.335	1.452
					341.7	1.342	1.336	1.453

					341.8	1.344	1.337	1.453
					342.0	1.345	1.338	1.454
					342.2	1.346	1.338	1.455
					342.4	1.345	1.339	1.456
					342.5	1.346	1.340	1.456
					342.7	1.346	1.340	1.457
					342.9	1.348	1.341	1.458
					343.1	1.349	1.342	1.458
					343.2	1.350	1.342	1.459
					343.4	1.354	1.343	1.460
					343.6	1.357	1.344	1.460
					343.8	1.359	1.344	1.461
					344.0	1.362	1.345	1.462
					344.1	1.365	1.346	1.462
					344.3	1.365	1.346	1.463
					344.5	1.365	1.347	1.464
					344.7	1.367	1.348	1.464
					344.8	1.369	1.349	1.465

					345.0	1.371	1.349	1.466

	Experimental Melting Point ^{o}C	Reported Melting Point ^{o}C
Glucose	158	150-152[1]
Maltose	122	102-103[2]
Trehalose	210	203-205[1]
Galactose	178	164-170[1]
Saccharin	231	224-230[1]
Sodium Cyclamate	263	265[3]-300[1]
Aspartam	220	231-249[1]

Appendix E: Liquid Isobaric Heat Capacity Database for Biofuels

Name	M [g.mol^{-1}]	α [mol.g^{-1}]	Database	T [K]	C_{pDS} [J.K^{-1}.g^{-1}]		
					Experimental	Calculated using Dadgostar-Shaw (DS)	Calculated using the heteroatom corrected DS (chap5)
Canola CB-01 oil	291.53	0.188	Test set 3	285.1	2.054	1.892	1.926
				287.3	2.060	1.901	1.935
				289.4	2.073	1.910	1.944
				291.6	2.079	1.919	1.953
				293.7	2.093	1.928	1.962
				295.9	2.103	1.937	1.970
				298.0	2.114	1.946	1.979
				300.2	2.128	1.955	1.988
				302.3	2.144	1.963	1.997
				304.5	2.157	1.972	2.005
				306.6	2.168	1.981	2.014
				308.8	2.180	1.989	2.023

				310.9	2.196	1.998	2.031
				313.1	2.208	2.007	2.040
				315.2	2.223	2.015	2.048
				317.4	2.237	2.024	2.057
				319.5	2.253	2.032	2.065
				321.7	2.267	2.041	2.074
				323.8	2.283	2.049	2.082
				326.0	2.299	2.058	2.090
				328.1	2.317	2.066	2.099
Canola I25 oil	293.17	0.190	Test set 3	286.1	2.067	1.908	1.942
				288.2	2.074	1.917	1.950
				290.3	2.080	1.925	1.959
				292.4	2.091	1.934	1.968
				294.6	2.101	1.943	1.976
				296.6	2.113	1.951	1.985
				298.7	2.126	1.960	1.993
				300.9	2.142	1.969	2.002
				303.0	2.159	1.977	2.011

				305.1	2.176	1.986	2.019
				307.2	2.191	1.994	2.027
				309.3	2.212	2.003	2.036
				311.4	2.231	2.011	2.044
				313.5	2.251	2.020	2.053
				315.6	2.272	2.028	2.061
				317.7	2.293	2.036	2.069
				319.8	2.315	2.045	2.077
				321.9	2.338	2.053	2.086
				324.0	2.360	2.061	2.094
				326.1	2.385	2.069	2.102
				328.1	2.412	2.078	2.110
Soy MG-B100 oil	291.27	0.188	Test set 3	283.1	2.157	1.886	1.920
				285.4	2.154	1.896	1.930
				287.6	2.157	1.905	1.939
				289.9	2.157	1.915	1.948
				292.1	2.161	1.924	1.958
				294.4	2.165	1.933	1.967

				296.6	2.167	1.942	1.976
				298.9	2.171	1.952	1.985
				301.1	2.176	1.961	1.994
				303.4	2.176	1.970	2.003
				305.6	2.183	1.979	2.013
				307.9	2.185	1.988	2.022
				310.1	2.188	1.997	2.031
				312.4	2.190	2.006	2.040
				314.6	2.192	2.015	2.049
				316.9	2.194	2.024	2.057
				319.1	2.199	2.033	2.066
				321.4	2.202	2.042	2.075
				323.6	2.207	2.051	2.084
				325.9	2.215	2.060	2.093
				328.1	2.224	2.069	2.101
Soy S-B100 oil	291.77	0.188	Test set 3	287.1	2.077	1.899	1.932
				289.2	2.081	1.907	1.941
				291.2	2.087	1.916	1.949

				293.3	2.092	1.924	1.958
				295.3	2.097	1.933	1.966
				297.4	2.104	1.941	1.975
				299.5	2.114	1.950	1.983
				301.5	2.121	1.958	1.991
				303.5	2.131	1.966	2.000
				305.6	2.141	1.975	2.008
				307.7	2.150	1.983	2.016
				309.7	2.158	1.991	2.024
				311.8	2.168	1.999	2.033
				313.8	2.177	2.008	2.041
				315.9	2.188	2.016	2.049
				317.9	2.200	2.024	2.057
				320.0	2.212	2.032	2.065
				322.0	2.220	2.040	2.073
				324.1	2.228	2.048	2.081
				326.1	2.238	2.056	2.089
				328.2	2.248	2.064	2.097

Rapeseed oil	294.56	0.189	Test set 3	287.1	2.214	1.908	1.941
				289.2	2.219	1.917	1.950
				291.2	2.229	1.925	1.958
				293.3	2.234	1.934	1.967
				295.3	2.241	1.942	1.975
				297.4	2.248	1.951	1.984
				299.5	2.255	1.959	1.992
				301.5	2.265	1.967	2.000
				303.5	2.272	1.976	2.009
				305.6	2.281	1.984	2.017
				307.7	2.290	1.992	2.025
				309.7	2.298	2.001	2.033
				311.8	2.308	2.009	2.042
				313.8	2.319	2.017	2.050
				315.9	2.329	2.025	2.058
				317.9	2.341	2.033	2.066
				320.0	2.354	2.041	2.074
				322.0	2.367	2.050	2.082

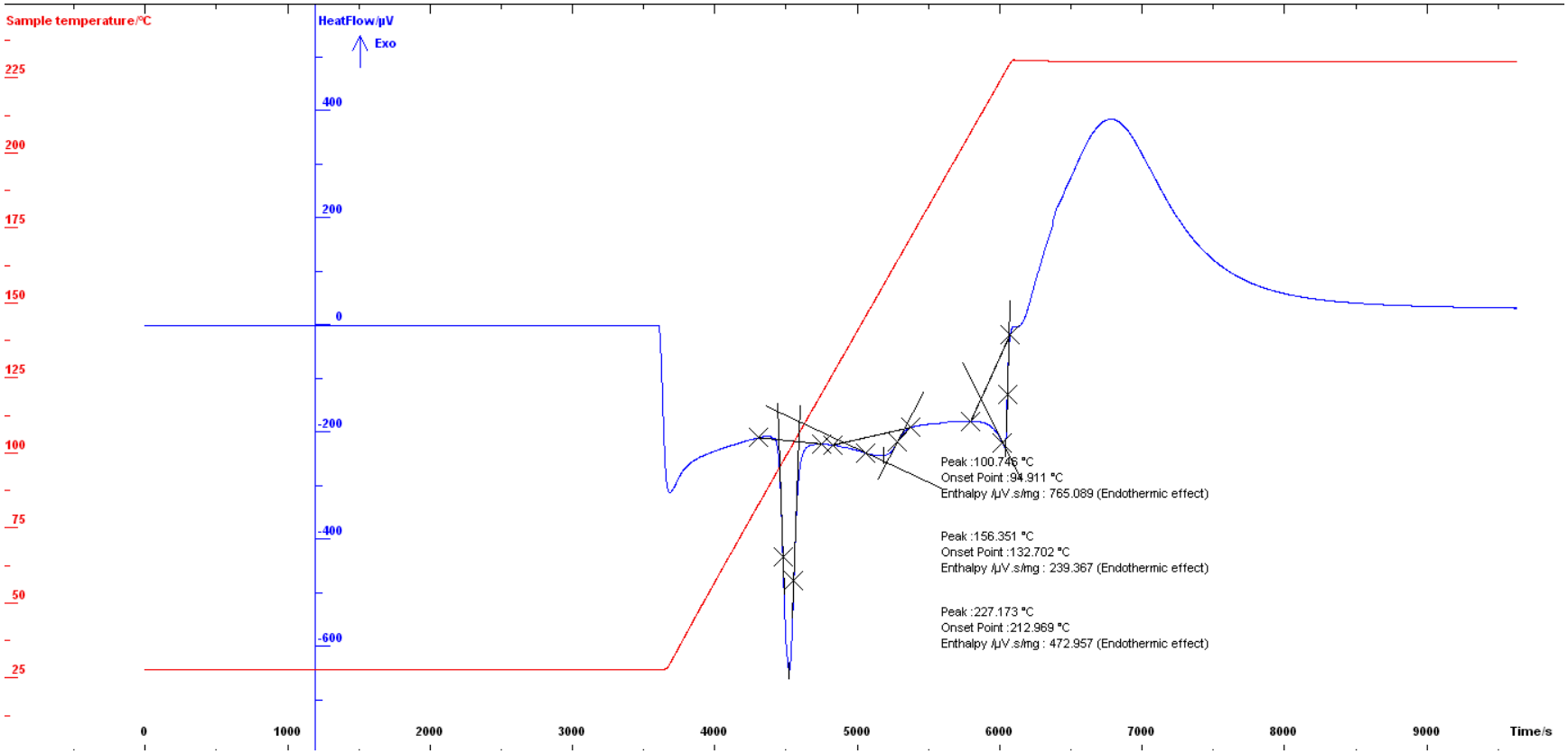
				324.1	2.380	2.058	2.090
				326.1	2.393	2.066	2.098
				328.2	2.407	2.074	2.106
Palm oil	283.69	0.193	Test set 3	297.1	2.083	1.968	2.003
				298.7	2.086	1.975	2.009
				300.2	2.105	1.981	2.016
				301.8	2.098	1.987	2.022
				303.3	2.110	1.994	2.028
				304.9	2.128	2.000	2.034
				306.5	2.136	2.006	2.041
				308.0	2.151	2.013	2.047
				309.5	2.168	2.019	2.053
				311.1	2.175	2.025	2.059
				312.7	2.182	2.031	2.065
				314.2	2.190	2.037	2.071
				315.7	2.202	2.043	2.078
				317.3	2.218	2.050	2.084
				318.9	2.227	2.056	2.090

				320.4	2.248	2.062	2.096
				321.9	2.246	2.068	2.102
				323.5	2.269	2.074	2.108
				325.0	2.288	2.080	2.114
				326.6	2.300	2.086	2.120
				328.1	2.319	2.092	2.126
Coconut oil	218.16	0.189	Test set 3	283.1	2.018	1.889	1.937
				285.4	2.023	1.898	1.946
				287.6	2.031	1.908	1.955
				289.9	2.040	1.917	1.965
				292.1	2.055	1.927	1.974
				294.4	2.054	1.936	1.983
				296.6	2.057	1.945	1.992
				298.9	2.067	1.955	2.002
				301.2	2.069	1.964	2.011
				303.4	2.073	1.973	2.020
				305.6	2.081	1.982	2.029
				307.9	2.085	1.991	2.038

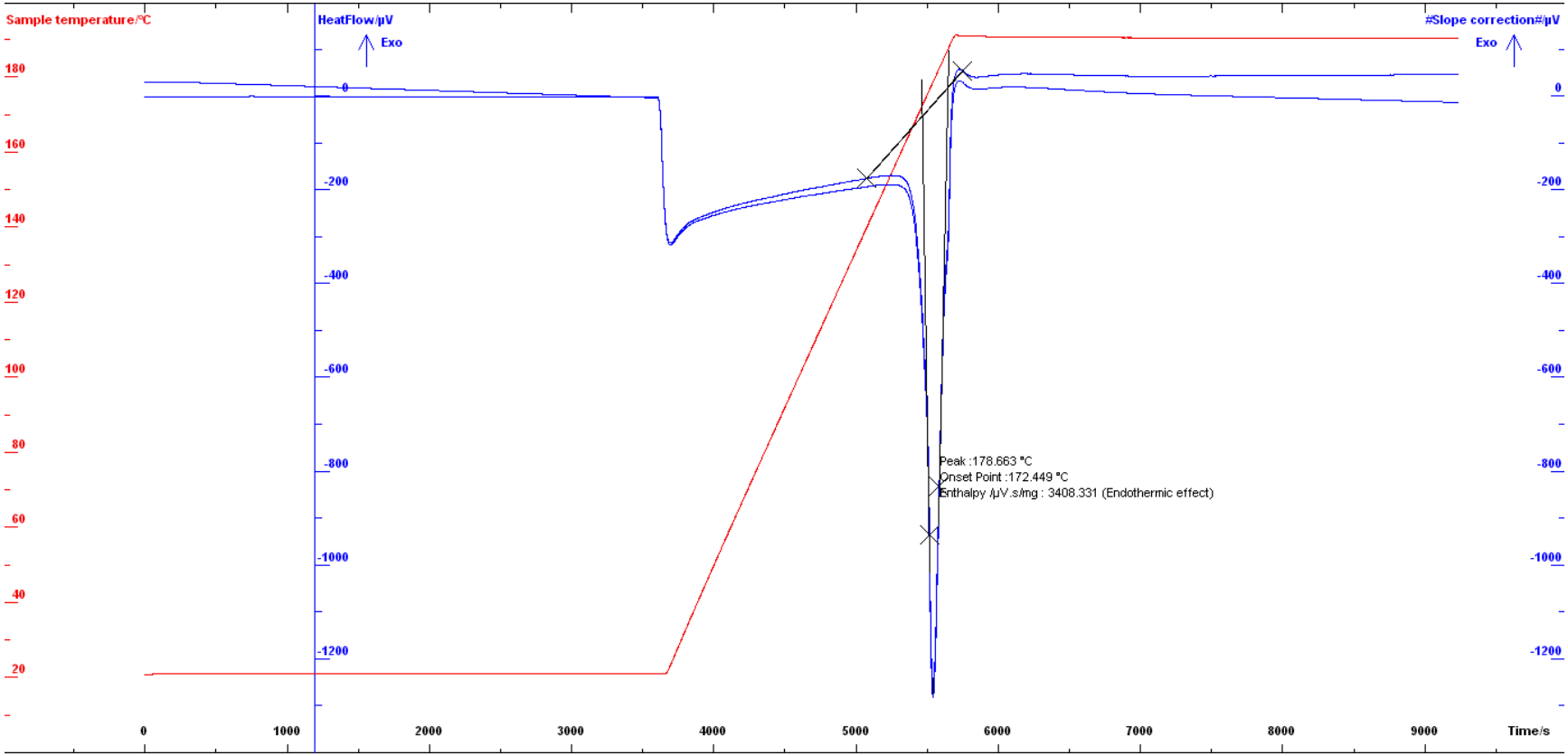
				310.2	2.093	2.000	2.047
				312.4	2.099	2.009	2.056
				314.7	2.110	2.018	2.065
				316.9	2.116	2.027	2.074
				319.2	2.126	2.036	2.082
				321.4	2.137	2.045	2.091
				323.7	2.148	2.054	2.100
				325.9	2.154	2.063	2.109
				328.2	2.161	2.071	2.117

Appendix F: Sugar DS Experimental data

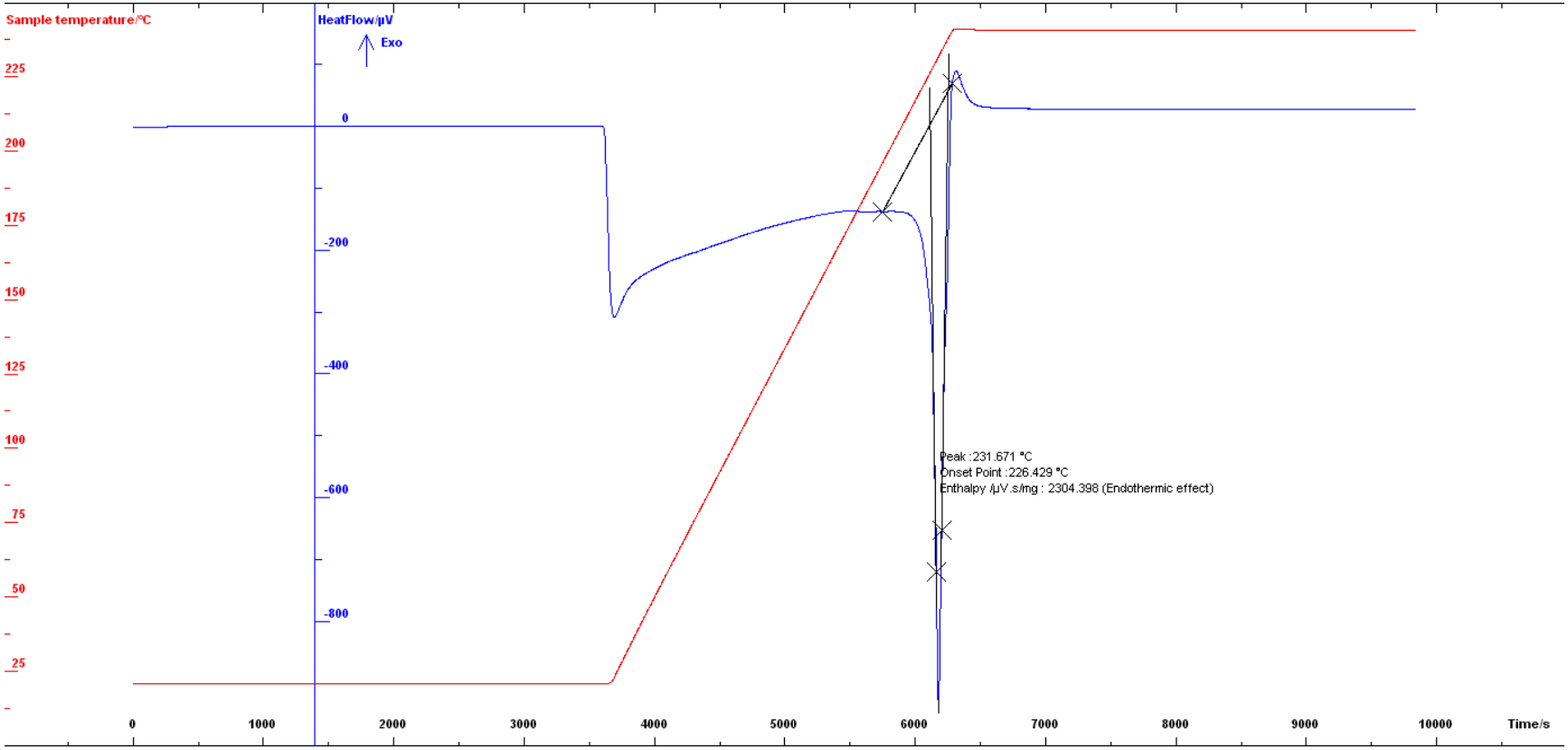
Trehalose



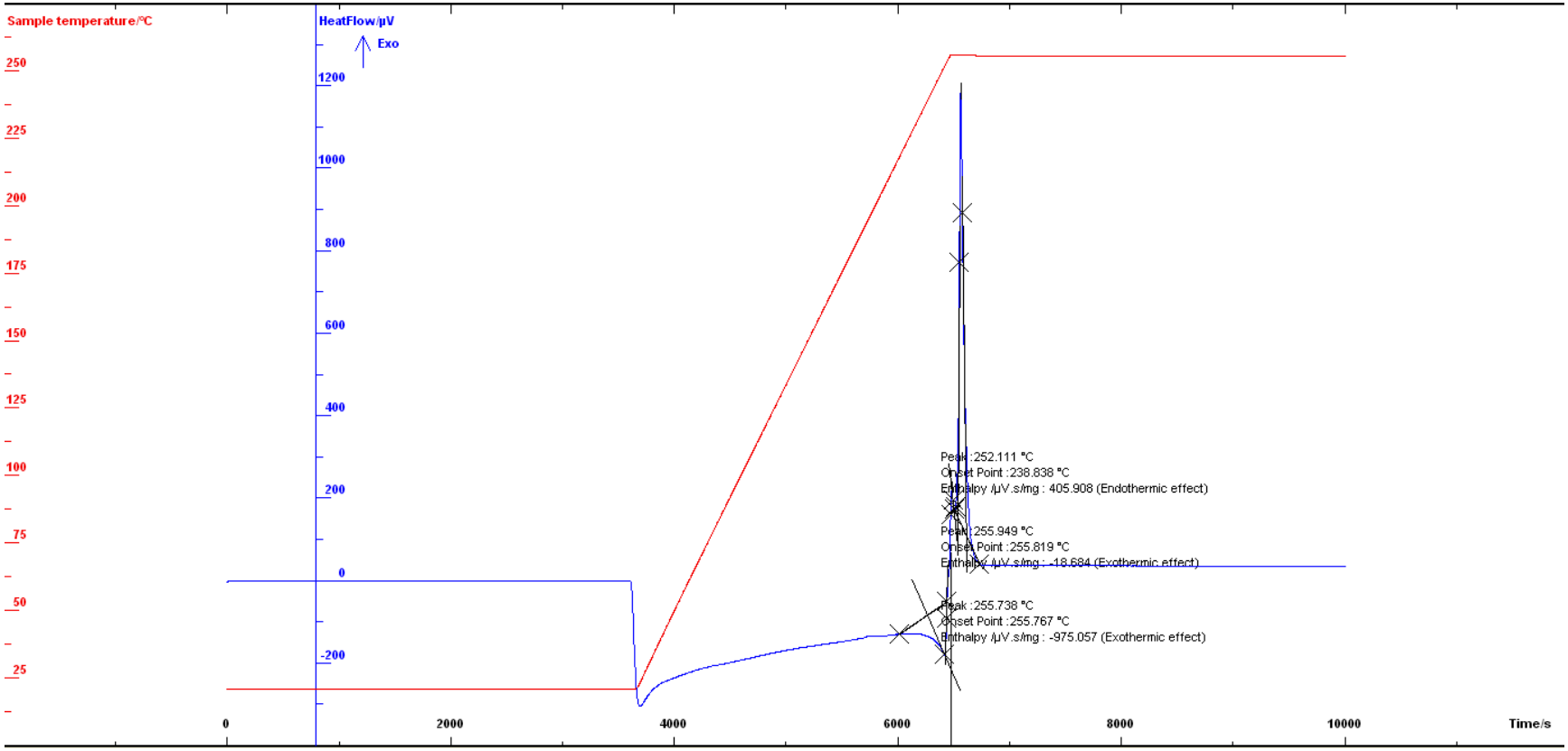
Galactose:


Sample temperature/°C
HeatFlow/µV
Exo
#Slope correction#/µV
Exo
Peak :178.663 °C
Onset Point :172.449 °C
Enthalpy /µV.s/mg : 3408.331 (Endothermic effect)
Time/s

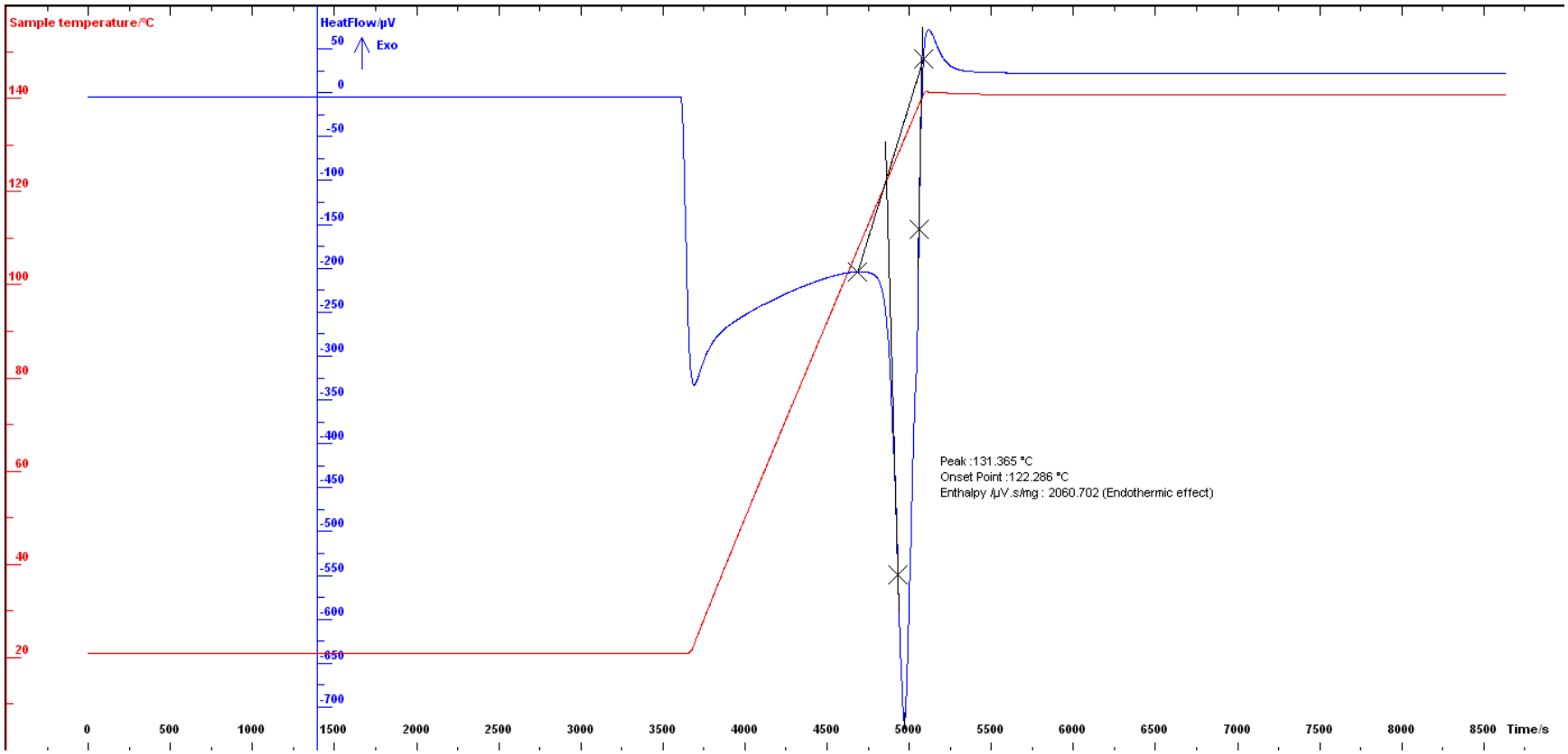
Saccharine


Sample temperature/°C
HeatFlow/µV
Exo
225
200
175
150
125
100
75
50
25
0
-200
-400
-600
-800
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
Time/s
Peak :231.671 °C
Onset Point :226.429 °C
Enthalpy /µV.s/mg : 2304.398 (Endothermic effect)

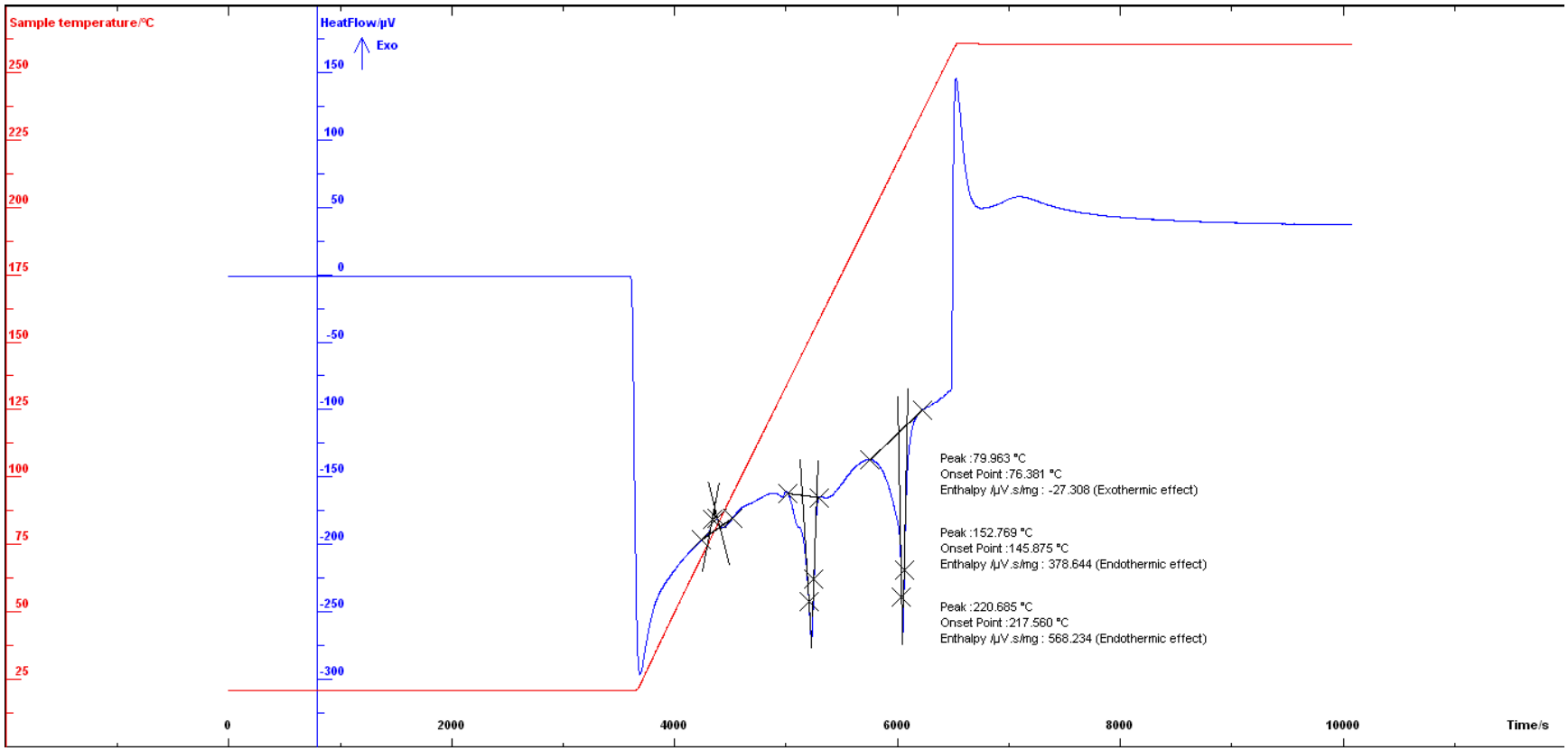
Sodium Cyclamate



Maltose


Sample temperature/°C
HeatFlow/µV
Exo
Peak :131.365 °C
Onset Point :122.286 °C
Enthalpy /µV.s/mg : 2060.702 (Endothermic effect)
Time/s

Aspartame


Sample temperature/°C
HeatFlow/µV
Exo
250
225
200
175
150
125
100
75
50
25
150
100
50
0
-50
-100
-150
-200
-250
-300
0
2000
4000
6000
8000
10000
Time/s
Peak :79.963 °C
Onset Point :76.381 °C
Enthalpy /µV.s/mg : -27.308 (Exothermic effect)
Peak :152.769 °C
Onset Point :145.875 °C
Enthalpy /µV.s/mg : 378.644 (Endothermic effect)
Peak :220.685 °C
Onset Point :217.560 °C
Enthalpy /µV.s/mg : 568.234 (Endothermic effect)