CRC Report No. RW-107-3a

VALIDATION OF THE NEW PM INDEX FORMULA: PHASE 2

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COORDINATING RESEARCH COUNCIL, INC.
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LIST OF ACRONYMS

AKI	Anti Knock Index
ASTM	American Society for Testing and Materials
CRC	Coordinating Research Council
DBE	Double Bond Equivalent
DHA	Detailed Hydrocarbon Analysis
DI	Direct injection (see SIDI)
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
E0	Gasoline that does not contain ethanol
E10	Gasoline containing 10 vol% ethanol
E15	Gasoline containing 15 vol% ethanol
E20	Gasoline containing 20 vol% ethanol
E>0	Gasoline containing ethanol at any level
EtOH	Ethanol Content
MAE	Maximum Absolute Error
MSS	Micro Soot Sensor
MW	Molecular Weight
NREL	National Renewable Energy Laboratory
PM	Particulate Matter
PME	PME (Particulate Matter Emissions) Index
PMI	Particulate Matter Index (Honda Equation)
PFI	Port Fuel Injection
R^2	Coefficient of Determination
RMS	Root Mean Square
RVP	Reid Vapor Pressure
SIDI	Spark-Ignition Direct-Injection (see DI)
SSI	Separation Systems, Inc.
SwRI	Southwest Research Institute
US	United States
VP_{443K}	Vapor Pressure at 443K
YSI	Yield Sooting Index

EXECUTIVE SUMMARY

Particulate matter (PM) emissions from gasoline vehicles and the relationship to fuel properties and composition continues to be a topic of research interest in automotive fuels and emissions. In prior work by CRC, EPA, and others, the Honda Particulate Matter Index (PMI) was used as a composition-based measure of a gasoline's potential to influence tailpipe PM emissions from vehicles, but without consideration of ethanol content, vehicle hardware, or engine design/calibration, all of which impact PM emissions. PMI is computed from a Detailed Hydrocarbon Analysis (DHA) performed according to the ASTM D6730 standard and variants thereof.

Beginning with CRC Projects AVFL-29 and RW-107, CRC has sponsored work to improve the quality of DHAs available to characterize gasoline composition and to develop an improved PM index to assess the impact of gasoline composition on PM emissions:

- CRC Project AVFL-29 focused on improved DHAs by extending the identification of gas chromatography peaks to cover more of the heavy hydrocarbons in gasoline. The work has been adopted in the current ASTM D6730-21 standard for DHA (see its Appendix A and Table X1.).

- CRC Project RW-107 examined the Honda PMI and several simplified, correlation-based indices to determine their efficacy in predicting LA92 Phase I[1] PM emissions. PMI was found to be a biased indicator when applied to groups of gasolines with varying ethanol content – i.e., E0 (neat) and E10 (10% ethanol by volume). PM emissions from gasoline with ethanol were found to be consistently greater than emissions from non-oxygenated gasoline of the same PMI.

- CRC Project RW-107-2 developed a "new technology" PM index—the PME (Particulate Matter Emissions) index—capable of indicating PM emissions potential for a broad range of gasolines. The Honda PMI correlation was originally developed using only neat gasolines but has been routinely applied to ethanol-containing gasolines. The PME was specifically designed for use with both neat and ethanol-containing gasolines up to E20. Further, it was designed to be directly proportional to LA92 Phase I PM emissions so that a percentage reduction in the index translates to the same percentage reduction in Phase I PM emissions from vehicles on average.

The current work, CRC Project RW-107-3a, was planned to validate the performance of PME using independent datasets of vehicle emissions during operation on a variety of gasolines. In doing so, revisions to its formulation were identified that would improve the index and extend its

[1] The cold-start phase during which the largest share of PM is emitted in both SIDI and PFI engines.

applicability to a wider range of gasolines. The revised (i.e., New) PME presented here is an improvement over the predecessor PME from RW-107-2 and should be used exclusively, as the predecessor is now obsolete.

Figure ES-1 summarizes the New PME index, both its mathematical form and the empirical coefficients needed to evaluate it for spark-ignition direct injection (SIDI) and port fuel injection (PFI) vehicles, the technologies that account for a dominant share of today's gasoline-fueled in-use fleet. PME is evaluated from a DHA determination of a gasoline's composition by hydrocarbon compound.

A variety of DHA procedures are used in US laboratories, including the current ASTM D6730-21 and earlier versions of the standard, many with local extensions made to expand the compound identification library. The New PME can be used with any ASTM-based DHA procedure that identifies a recommended 98 percent or more of a gasoline by weight (wt%) as specific compounds or as groups of related isomers. The PME values calculated from a DHA are standardized (by statistical expansion) to estimate the index value corresponding to 99.9 wt% identification of the compounds in gasoline, the highest coverage reached using the current ASTM DHA standard.

Figure ES-1
The New PME Formulation

Direct Proportionality (1.0)

$$\text{LA92 Phase 1 PM} = A_{Veh} \cdot PME_{Eng\ Tech}$$

Empirical parameters are in orange.

$$PME = \left(\frac{43.4}{LHV}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot YSI_i}{VP_i^{\alpha=f(EtOH)}} \right]^{(1+\beta\cdot(99.9-FuelCoverage_{DHA}))}$$

$$\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$$

$$f(EtOH) = \alpha_{E0} + \Delta\alpha \cdot EtOH_{VOL\%}$$

$FuelCoverage_{DHA}$ = Total Wt% Identified in DHA

LHV = Lower Heating Value

Engine Technology	DHA Type	N_{TECH}	α_{E0}	α_{E10}	α_{E15}	α_{E20}	β
SIDI	ANY	0.001025	0.451	0.430	0.419 a/	0.409 a/	0.122
PFI	ANY	0.000558	0.257	0.250	0.236	0.222	0.122

a/ Recommended extension to E15 and E20 based on the α_{E0} to α_{E10} trend.

Strengths of the New PME compared to the Honda PMI and other PM indices are the following:

- It correlates well with Phase I PM emissions over the full range of E0 through E20 gasolines. The direct proportionality between PME and Phase I PM emissions means that users can be confident that percentage reductions in the index will translate into the same or larger percentage reductions in PM emissions for a fleet of vehicles on average.
- It more accurately accounts for the chemical sooting potential of the gasoline by incorporating the Yield Sooting Index (YSI) in place of the double bond equivalents employed in the PMI calculation. YSI was quantified at Yale University and developed at the National Renewable Energy Laboratory (NREL) to characterize soot formation from individual hydrocarbons and oxygenated compounds found in gasoline and bio-fuels;
- It accounts for the extent that vaporization before combustion enriches fuel droplets (and localized areas with rich air-fuel ratios) in heavy hydrocarbons due to the faster vaporization of the lighter compounds;
- It accounts for the manner in which ethanol accelerates the vaporization of itself and other compounds in a gasoline, cooling the fuel charge and leading to its further enrichment in heavy hydrocarbons; and
- It accounts for the manner in which changes in the energy density of gasoline influence the quantity of fuel needed to propel a vehicle and, thus, its PM emissions in terms of the PM mass emitted per unit distance.

Organizations that want to use PME in research or fuel blending can obtain an Excel-based PME calculator from CRC along with a guide to its use. The calculator will determine the Honda PMI and the New PME indices for SIDI and PFI vehicles from a DHA input by the user. The calculator recognizes all compound identifications in Table X1.2 of the ASTM D6730-21 DHA standard along with additional compounds that are found in DHAs performed (according to earlier versions of the standard) for a number of PM emission studies.

1. INTRODUCTION

1.1 Background and Objectives

Automotive engine technology has changed substantially in the past two to three decades under the influence of increasingly stringent tailpipe emissions and fuel economy standards in the US and other countries. Carburetors have been replaced with Port Fuel Injection (PFI) systems to permit precise control of the air-fuel mixture and, more recently, with technologies such as the Spark Ignition Direct Injection (SIDI) engine. SIDI engines use sophisticated computer control and in-cylinder injectors to deliver atomized gasoline directly into the cylinder (rather than the intake manifold) in an effort to maximize engine output and minimize fuel consumption.

Combustion in gasoline engines can produce particulate matter (PM) in localized areas with rich air-fuel ratios or when heterogenous combustion involving liquid fuel droplets occurs. In PFI engines, this occurs mainly during cold-start—for example, pool fires from liquid fuel accumulation on combustion system surfaces—and is greatly diminished once the engine becomes fully warm. In SIDI engines, this occurs in appreciable amounts throughout all phases of driving, although the largest share of PM is still emitted during cold start operation. PM emissions from SIDI vehicles have historically been higher than from PFI vehicles, although some modern SIDI designs, such as those utilizing high pressure fuel injection systems with minimum wall wetting, have demonstrated comparable emissions (Saliba 2017).

Honda was the first to introduce a Particulate Matter Index (PMI) that relates the chemical composition of a gasoline to the PM emissions from vehicles (Aikawa 2010). The PMI is based on a profile of the individual hydrocarbons in a gasoline as determined through a Detailed Hydrocarbon Analysis (DHA), typically using the ASTM D6730 procedure. DHAs generated from variants of the ASTM procedure also have been used to determine PMI for fuels.

Given a DHA, the PMI for a gasoline is calculated using the Honda Equation:

$$\text{PMI} = \sum_i Wt_i * \left(\frac{1+DBE}{VP \text{ at } 443K} \right) \quad (1\text{-}1)$$

Here, the summation is over the compounds identified in the DHA, $Wt\%_i$ is the weight fraction for each, DBE_i is the count of double-bonds and their equivalents in the form of triple bonds and rings in each compound, and VP_i is the vapor pressure at 443K. The numerator 1+DBE was adopted as the indicator of a compound's propensity to soot based on the research available at the time.

The Honda PMI and several simplified, correlation-based PM and soot indices were evaluated in CRC Project RW-107 to determine their performance in predicting the relative PM emission trends of gasolines. PMI was found to perform well *if* the gasolines shared the same ethanol content, but

it proved to be a biased indicator when applied to mixed groups of neat (E0) and ethanol-containing gasoline (E10, E15, E20). LA92 Phase I PM emissions from the ethanol-containing gasolines were found to be consistently greater than emissions from neat gasoline of the same PMI[2].

To fill the need for a PM index that would indicate the PM emissions potential for a broad range of gasolines, CRC Project RW-107-2 examined alternative mathematical formulations for a PM index. The objective was to eliminate the Honda PMI's ethanol bias and to create a "new technology" PM index that could serve fuel research and gasoline blending into the future. The result of that work was the PME (Particulate Matter Emissions) index, an indicator of PM emissions over Phase I of the LA92 test cycle.

The current project, CRC Project RW-107-3a, was initiated to validate the PME index developed in RW-107-2 using PM emissions datasets not considered in its development. The datasets included new testing performed by Southwest Research Institute (SwRI) in CRC Project RW-107-3 and testing from a 2018 study funded by Growth Energy that was conducted at the UC Riverside CE-CERT emissions testing facility. The validation analysis showed generally satisfactory performance for the PME index, but also the possibility of improvement in select areas. Further analysis was then performed to create a revised version of PME that replaces the original PME developed in CRC Project RW-107-2.

Sections 2 and 3 discuss the validation of the PME index developed in RW-107-2. Use of the term PME in those sections refers exclusively to the RW-107-2 PME. Beginning with Section 4, the report turns to the revised PME developed in the second phase of this work (RW-107-3a). The RW-107-2 PME is referred to as the original or Old PME. The PME developed here is referred to as the revised PME or the New PME.

1.2 Report Organization

Section 2 gives a brief summary and review of the PME formulation developed in RW-107-2, including its mathematical form and conceptual underpinnings. It identifies the areas in which it is revised in the current work to give the reader orientation to the chief issues addressed.

Section 3 presents the results of the validation analysis conducted to understand the performance and applicability of the PME index when applied to new datasets not used in its development. The work also gives the opportunity to observe its performance when applied to the emissions of PFI and SIDI vehicles certified to Tier 3 emission standards instead of the Tier 2 vehicles in the datasets used for its development.

Section 4 presents the work done to revise the PME index to improve its performance and applicability to a wider range of gasolines. The major revisions are these:

- A statistical approximation of the Yield Sooting Index (YSI) in the numerator of the PME is replaced with the measured and estimated YSI values by compound that the approximation represented.

[2] CRC Project RW-107 (2019), Assessment of the Relative Accuracy of the PM Index and Related Methods. CRC Project RW-107. April 2019.

- The PME formulation is recast to expand the index value that is computed from the DHA, which vary across gasolines and laboratories in terms of the wt% coverage of the fuel, to estimate the index value at a reference DHA coverage of 99.9 wt%. The reference coverage of 99.9 wt% is the highest that has been achieved for the experimental fuels considered here using the current ASTM D6730-21 standard.

Scaling of PME with respect to the Honda PMI is also discussed along with the methods used to re-estimate PME.

Section 5 presents the New PME with its empirical coefficients. Key features of its mathematical formulation are explained and its performance is demonstrated for the datasets used for its development and validation. Section 6 completes the analysis by comparing the New PME and Honda PMI with respect to four different aspects of their relationship and performance as indicators of PM emissions.

Section 7 provides a summary and discussion of the work presented here.

Three appendices are included to document the work in this project:

- Appendix A contains the SWRI report on the vehicle testing conducted under CRC Project RW-107-3 to support this work.
- Appendix B contains a master list of information on hydrocarbons compounds that will be needed by potential users interested in evaluating the New PME for their gasolines. It includes the YSI value for each compound along with updated and standardized data on boiling point (BP) and vapor pressure at 443K (VP_{443K}) as used here and recommended for use.
- Appendix C tabulates the New PME index values for each experimental gasoline in the CRC studies used in this work.

Supplementary material for this work is available from CRC, including the following:

- An Excel version of the master list of hydrocarbon compounds contained in Appendix B (CRC Project RW-107-3a AppB.xlsx). This includes additional information on the compounds beyond that shown in Appendix B.
- An Excel-based PME calculator with user notes that can be used by interested parties to evaluate the Honda PMI and the New PME index of gasolines for which DHAs have been performed.

2. REVIEW OF THE RW-107-2 PME FORMULATION

2.1 Overview

The mathematical formulation of the original PME index, developed in RW-107-2, is given in Equation 2-1 for comparison to the Honda PMI given in Equation 2-2. In both cases, the summation is computed over the individual compounds *i* that are identified as present in a gasoline by the DHA. As is customary, the wt%$_i$ parameter is in percentage terms—1.0 wt% is written as 1.0 in calculations.

$$\text{PME} = \left(\frac{43.4}{\text{LHV}}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(\text{EtOH})}} \right]^{\beta} \qquad (2\text{-}1)$$

$$\text{PMI} = \sum_i \frac{wt\%_i \cdot (1+DBE)_i}{VP_i} \qquad (2\text{-}2)$$

Green font is used in Eq. 2-1 to show the empirical terms that contribute to PME. The Honda PMI, Eq. 2-2, was framed as written based on the experimental evidence available in 2010 regarding how selected properties of compounds contribute to PM emissions formation. It was written without empirical terms and was evaluated using a dataset of gasolines that did not contain ethanol (Aikawa 2010).

The boxed portion of the PME equation re-writes the summation of the Honda PMI to improve the characterization of each compound's propensity to form PM emission when combusted. In the numerator, the quantity yTerm$_i$ is a simplified estimator of each compound's sooting propensity that can be calculated from counts of bonds and rings in the molecule. It is a statistical representation of measured sooting values in the YSI Version 2 Database (Das 2018). In the denominator, the $1/VP^{\alpha}$ term is a generalization of the 1/VP term in the Honda PMI that allows each compound's contribution to PM to vary from the simple inverse-proportionality to vapor pressure. The α exponent depends upon the engine's fuel injection method (SIDI or PFI) and the gasoline's ethanol content. The α exponent was empirically estimated from analysis of PM emissions in the CRC E-94-2 study (for SIDI vehicles) and the EPAct study (for PFI vehicles).

Outside the summation term, a normalization factor N_{TECH} causes the PME and PMI values to coincide at an index value of 1.00[3]. The factor differs between SIDI and PFI technologies because the α exponent in the denominator differs between those groups. However, the factor does not, itself, represent vehicle technology effects such as engine efficiency, vehicle size, fuel injection pressure, injector placement (central or side), or combustion system design. The

[3] That is, a fuel with a PME value of 1.00 can be expected to have Honda PMI of 1.00 as well.

portion of PME in square brackets ("[…]") can be viewed as an enhancement of the Honda PMI equation. Like PMI, it is stated on a weight basis—*per kg of fuel*—because wt% is used in the calculation.

Outside the square brackets, an exponent β "grosses up" the computed index value to account for the lower compound identification rates when PME is evaluated using an earlier version of ASTM D6730 standard. When the DHA is performed using the current D6730-21 version (which implements an enhanced procedure developed in CRC AVFL-29), the β coefficient has value 1.00 and has no effect on the computed value. When evaluated using *any* earlier version of the standard, the β coefficient has the value 1.17. Thus, the PME formulation recognized two classes of DHAs: the current D7630-21 version (an "SSI" DHA) and any done according to one of the earlier versions (an "ASTM" DHA).

Finally, PME adds a term in front that adjusts the PM propensity of the fuel to reflect that more kg's of a fuel must be burned to power a vehicle over a given test cycle or real-world trip if it has a lower energy content per kg, as oxygenated gasolines typically do. Thus, a gasoline's propensity to form PM emissions is more than just the propensity of its composition. Energy content is measured as Lower Heating Value (LHV) in units of MJ/kg of fuel. The reference value of 43.4 MJ/kg was chosen as representative of conventional or reformulated gasoline not containing ethanol or another oxygenate (GREET 2019).

2.2 Concepts Behind YSI

In the Honda equation, the 1 + DBE term represents the difficulty of breaking a molecule's double and higher bonds, which can be thought of, in a generalized sense, as its "stability." The Double Bond Equivalent (DBE) simplifies multiple types of bonds—including double bonds, triple bonds (which are doubly weighted), and rings—into an equivalent number of double bonds. Single bonds are not considered in this determination because of their ease of breaking. The leading term 1 represents a contribution from saturated compounds while DBE represents an additional contribution from non-saturated compounds. Compounds with a larger number of stable bonds (higher DBE) are more likely to form PM when combusted.

Both the original PME and the revised PME developed here use the YSI as the basis for estimating a compound's inherent sooting potential. The Pfefferle Lab Group at Yale measured the soot (PM) formed by pure hydrocarbon compounds, including oxygenates, when combusted in a methane diffusion flame. From this, the YSI Version 2 Database was developed as a standardized measure of soot formation potential. The database contains YSI values on a unified scale and stated on a mole basis (a constant molar concentration in the flame). Although collected under combustion conditions that differ from those in a vehicle engine, YSI values characterize the way in which compounds actually react during combustion to form soot and PM. YSI is an empirical measure for the many compounds tested; for those not measured, an estimated YSI is available, based not only on numbers and types of bonds present but also on consideration of the intermediate pathways by which the compounds break down during combustion (Das 2018). Therefore, YSI is expected to be a better metric than DBE for indicating the relative PM forming potential of different gasolines based on their detailed chemical composition.

While hundreds of compounds have been measured, the YSI work was motivated in part by the need to characterize the sooting potential of bio-based and blended petroleum-biofuels. As a result, the YSI database contains many compounds that are not found in commercial gasolines today—specifically, many complex oxygenates such as ketones, aldehydes, and other compounds with multiple oxygen groups. Only 131 of the 860 compounds found in the experimental gasolines were contained in the YSI database.

The YSI-based approach was adopted at a time when it was not possible to gauge its ultimate success or the cost-effectiveness of estimating[4] YSI values for all compounds. Instead, the $yTerm_i$ quantity was developed in RW-107-2 as a statistical approximation of the measured YSI values for the 131 overlapping compounds and used to extrapolate YSI to the full slate of hydrocarbons in the experimental gasolines. The $yTerm_i$ approximation is based on counts for bonds and rings in each molecule.

The New PME developed in this project replaces the $yTerm_i$ approximation with measured and estimated YSI values for all compounds found in the current D6730-21 standard for DHA plus those from earlier versions of the standard that were found in experimental gasolines. The assistance of Peter St. John and others at the National Renewable Energy Laboratory in this is gratefully acknowledged. See Section 4.2 for a description of YSI and its incorporation in the New PME.

2.3 The 1/VPα Denominator in PME

The authors of the Honda PMI noted that experimental evidence showed the contribution of individual compounds to be inversely proportional to their vapor pressure at 443K, but that the evidence did not give them a basis to select a specific functional form. The Honda Eq.'s denominator was made inversely proportional to VP_{443K} by assumption.

PME changes the denominator to allow an empirically determined exponent α to fine tune the role of vapor pressure. Vapor pressure spans more than three orders of magnitude across the compounds present in the experimental gasolines—from a low of 3 kPa for some C12-14 hydrocarbons to a high of 16,957 kPa for propene. Given this wide range, a power-law relationship of the form $1/VP^{\alpha}$ was a logical and suitable choice. The PME formulation is repeated below for reference.

$$\text{PME} = \left(\frac{43.4}{\text{LHV}}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=f(\text{EtOH})}} \right]^{\beta} \qquad (2\text{-}3)$$

The α term in the denominator represents how vaporization processes before combustion modify the chemical composition of the fuel that remains in the liquid state when combustion begins. At the outset, it was expected that α would depend on engine technology as PFI and SIDI vehicles differ greatly in the time allowed for injected fuel droplets to be heated and vaporized. PFI engines with fuel injection at the intake port allow an extended time for droplets

[4] Note that YSI can be estimated for other compounds using an online calculator developed by NREL and found at https://ysi.ml.nrel.gov/. The calculator accounts for a variety of factors influencing YSI including molecule structure, branching and pathways for breakdown during combustion.

to vaporize and the fuel charge to mix during the intake stroke before combustion begins. SIDI engines inject fuel directly into the cylinder during combustion, giving much less time for vaporization and mixing. It was also expected that ethanol content would influence the α values through its substantial effect on accelerating vaporizing during the early portions of the distillation curve. Both expectations were confirmed in the empirical analysis.

2.4 Energy Content Term

The leading term in PME represents the effect of varying energy content (due to gasoline composition) on the PM emissions realized from a vehicle. Because the summation term in PME gives a value stated on a weight basis—i.e., the gasoline's propensity to form soot per kg of fuel combusted—the energy content term was introduced to account for the fact that more kilograms must be consumed per mile if the energy content per kg is lower. The numerator 43.4 MJ/kg is a reference value for energy content that is representative of conventional or reformulated gasoline without ethanol. In this study, with few exceptions, only ethanol-containing gasolines are appreciably lower than 43.4 MJ/kg.

The need for the term can be understood by a simple thought experiment. Assume for illustration that ethanol has no effect on PM emissions other than to dilute the gasoline hydrocarbons. If 10 wt% ethanol is added to an E0 gasoline, the PM formation potential per kg of fuel is also reduced by 10%. However, the blended gasoline will contain about 3.5% less energy than before so that 1/(1-0.035) = 1.036 times as much blended gasoline must be consumed to propel the vehicle over the test cycle. Compared to PM emissions on the E0 gasoline, the emissions from the blended gasoline are reduced, not to 0.90 due to dilution, but to (1 - 0.10)·1.036 = 0.93 instead.

Individual vehicles may respond differently to gasolines and may use some gasolines more (or less) efficiently than others. In such case, the actual emissions change due to energy content will differ somewhat by vehicle. However, this is a *vehicle response* factor and not one that can be incorporated in an index describing *gasolines*.

2.5 Linearity of PME with LA92 Phase I PM Emissions

A design objective for PME was that its value should be linearly related—perhaps better stated as directly proportional—to the general trend of LA92 Phase I PM emissions of vehicles operated on different gasolines. Directly proportional means that a 10% increase or reduction in the PME index should result, on average, in a 10% increase or reduction in Phase I PM emissions for a fleet of vehicles. For the Honda PMI, Phase I PM emissions change more slowly than the calculated index value, so that a 10% reduction in PMI decreases Phase I PM emissions by only about 5%. The designed direct proportionality of PME holds for the Tier 2 PFI and SIDI vehicles used in its development, but may not hold for Tier 3 and later vehicles if substantial engine modifications have been made to reduce PM formation. The validation analysis tests this for Tier 3 vehicles.

The expected relationship between PM emissions and PME for gasoline *i* and vehicle *k* is as follows:

$$PM_{i,k} = A_k \cdot PME_i = A_k \cdot \left(\frac{43.4}{LHV}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=\alpha 0+\Delta\alpha\cdot EtOHvol\%}} \right]^1 \quad (2\text{-}4)$$

where A_k is the PM emissions response coefficient of vehicle k to PME, or equivalently, the PM emissions of the vehicle for a gasoline with PME = 1.00. The exponent to VP has been written out as $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ to explicitly show the effect of varying ethanol contents. For fuels research, the emissions response factors A_k can be determined in a regression or similar statistical analysis of PM emissions versus the index value. However, they need not be known for gasoline blending if the objective is to achieve percentage reductions in PM emissions through comparable reductions in PME.

2.6 Summary

Table 2-1 lays out the elements of PM formation in vehicles to show where and how they are represented in PME. Two elements are vehicle factors that influence A_k in Eq. 2-4 that must be accounted for in PM emissions analysis. Four are fuel factors that PME accounts for. The PME formulation accounts for the major elements of PM formation in vehicles as presently understood by the research community.

The $\Delta\alpha$ coefficient in $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ represents ethanol's cooling of the fuel charge that results from its higher Heat of Vaporization compared to gasoline hydrocarbons and its tendency to accelerate vaporization of other gasoline hydrocarbons by forming near-azeotropes with them. The near-azeotrope formation accelerates the vaporization of fuel fractions and depresses front-end distillation temperatures in ethanol-containing gasolines, which results in substantial cooling of the fuel charge. In turn, the cooling leaves the remaining fuel droplets and localized rich air-fuel ratios enriched in heavy hydrocarbons.

At present, the $\Delta\alpha$ coefficient in $\alpha = \alpha_0 + \Delta\alpha \cdot EtOH_{vol\%}$ is used only for ethanol and not for other oxygenates. Oxygenates differ in their Heats of Vaporization and their ability to form near-azeotropes and, thus, their tendency to influence fuel vaporization. The work reported in Fioroni 2019 illustrates these differences.

In the studies available to RW-107-2 and this project, only CRC Project E-129 examined other oxygenates, specifically i-Butanol and MTBE. Its small test fleet (4 vehicles) and use of fuels with low PM formation potential does not permit a meaningful test of PME performance for the other oxygenates. When PME is applied to fuels blended from oxygenates other than ethanol, the $\Delta\alpha$ coefficient should be set to zero. If PM emissions data are available for the fuels, a test should be applied to determine whether the observed emissions level of such fuels are different from that indicated by PME.

Table 2-1
PME and the Elements of PM Formation in Vehicles

Element	How Represented in PM Emissions Analysis and the PME Formulation	Discussion
Vehicle Factors (Accounted for in Emissions Analysis)		
Fraction of gasoline in fuel droplets or localized rich air-fuel ratios during LA92 Phase I.	Intercept terms for the average emission levels of vehicles.	Differs between SIDI and PFI vehicles.
Vehicle efficiency varies per kg of fuel. Vehicle emissions response varies by fuel.	Intercept terms for the average emission levels of vehicles. Increased residual error in the emissions analysis.	Vehicle specific, if present.
Fuel Factors (Accounted for in PME Index)		
Chemical propensity of the gasoline composition to produce soot.	YSI-based *yTerm* in numerator.	Influenced by the mix of gasoline hydrocarbons and ethanol or other oxygenates.
Early vaporization of light compounds leaves fuel droplets and localized rich air-fuel ratios enriched in heavy compounds.	$1/VP^{\alpha}$ term through the α_0 coefficient for E0 gasolines.	Differs between SIDI and PFI vehicles.
Accelerated vaporization of the fuel charge resulting from ethanol's presence leads to further enrichment.	$1/VP^{\alpha}$ term through the $\Delta\alpha$ coefficient for E>0 gasolines.	Differs between SIDI and PFI vehicles and as a function of ethanol content.
Reduced energy content per kg of fuel when ethanol or other oxygenates are present.	43.4/LHV term.	Permits PME to adapt to different oxygenates.

3. VALIDATION OF THE RW-107-2 PME FORMULATION

3.1 Introduction

The first objective of this project was to test the performance of the PME index developed in RW-107-2 against new datasets that had not been used in its development. This would determine how well it worked to indicate PM emissions when applied to gasolines not previously encountered and, where possible, from vehicles not previously tested during CRC Project E-94-2. The second objective was to expose areas, if they existed, where the index's performance could be improved.

One opportunity for this was as an offshoot of planned testing of a Portable Emissions Measuring System (SWRI) at the SwRI laboratory under CRC Projects E-122-2 and E-133. Under CRC Project RW-107-3, CRC made funds available to collect gravimetric PM measurements during Phase I of the LA92 test cycle that would be used for vehicle pre-conditioning. The resulting dataset is referred to in this report as the "SwRI" dataset. It contains the gravimetric measurements of Phase I PM emissions made to support the PME work, but not the PEMS and other measurements made for the original projects.

A second opportunity came with a 2018 study of vehicle emissions sponsored by Growth Energy, the leading biofuel trade association in the U.S., and conducted at the UC Riverside CE-CERT emissions testing laboratory. The organization granted access to the original emissions test data and analyses of the experimental gasolines so that a detailed analysis could be conducted in the manner done for the SWRI dataset and the preceding studies beginning with CRC Project E-94-2.

The following sections review the two validation datasets in further detail, followed by the presentation of the key results on PME performance for each. The final section summarizes what was learned about PME.

3.2 Vehicle Emissions Datasets

3.2.1 The SWRI Dataset under CRC Project RW-107-3

In the planned testing under CRC Projects E-122-2 and E-133, an LA92 test cycle would be used for vehicle conditioning before testing the PEMS system. Emissions collection and gravimetric measurement could be added to the test sequence at relatively low cost to obtain Phase I PM emissions to support this project. Appendix A contains SwRI's final report on the testing it conducted and can be consulted for additional information on the test procedures, characteristics of test vehicles and experimental gasolines and overall emission results.

The test fleet consisted of four vehicles, summarized in Table 3-1. One (Vehicle B), was a MY 2013 SIDI vehicle with direct-injection (DI) that had been tested previously in CRC E-94-2 and related projects. The other three (Vehicles A, C, and D) were more-recent MY 2019 PFI vehicles obtained locally by SwRI. The latter are the first vehicles certified to a Tier 3 emission standard that have been examined in the CRC projects leading up to the current one. PME was developed in RW-107-2 using Tier 2 SIDI vehicles from CRC E-94-2 and Tier 2 PFI vehicles from the EPAct study.

Table 3-1
Test Vehicles of the SWRI Dataset

PME Group	**SIDI**	**PFI**		
Vehicle	**B**	**A**	**C**	**D**
Year	2013	2019	2019	2019
Engine Type	DI Turbo	PFI NA	PFI NSA	PFI NA
Transmission	6-speed AT	6-speed AT	9-speed AT	e-CVT
Gasoline Type	Regular	Premium (recommended)	Regular	Regular
Start/Stop	No	No	Yes	Hybrid
EPA Cert	T2B5 LDV	T3B125 LDV	T3B30 LDT	T3B30 LDV
CA Cert	ULEV II PC	ULEV125 PC	SULEV30 LDT	SULEV30 PC
Source: Table 2. *CRC Project RW-107-3: Validation of the New PM Index Formula*. Southwest Research Institute. April 2023.				

A total of 13 experimental gasolines were used in the testing, as summarized in Table 3-2. The first nine gasolines (A-I) were selected according to the experiment design for Project E-122-2. One (Fuel A) was an EPA Tier 3 certification fuel with 10 vol% ethanol. Four gasolines (B-E) were E10 gasolines found in the commercial market to fill a 2 x 2 matrix of summer vs. winter RVP and High vs. Low PMI characteristics. Four more gasolines (F-I) were created by splash-blending additional ethanol into Fuels B-E to reach the E15 level. These were the gasolines used in the testing of the SWRI device under E-122-2 and E-133.

Four gasolines were added for the additional testing under RW-107-3 and used only to obtain LA92 Phase I PM emissions for this study. Fuels J and K were Summer High PMI and Winter Low PMI E10 gasolines. Fuels L and M were created by splash-blending additional ethanol with Fuel J to reach the E15 level.

This dataset provides the opportunity to see, for the first time, the performance of PME in a SIDI vehicle for winter gasolines (RVP 13-15 psi) and at ethanol levels up to E15. The CRC E-94-2 dataset on which the PME was based contained only RVP 7 psi gasoline at E0 and E10 levels. For the three PFI vehicles, the 13 experimental gasolines give a fresh look at the effects of RVP and ethanol up to E15 for Tier 3 PFI vehicles, in contrast to the much earlier model year Tier 2 PFI vehicles tested in the EPAct study.

Table 3-2
Experimental Gasolines of the SWRI Dataset

Fuel	Description	RVP (psi)	Ethanol (vol%)	Honda PMI	Description
A	Tier 3 Certification	9.2	9.7	1.71	EPA Tier 3 EEE
B	Summer Low	9.0	9.7	1.10	Market Fuel
C	Summer High	7.7	9.5	1.88	Market Fuel
D	Winter Low	15.3	9.6	0.67	Market Fuel
E	Winter High	13.6	10.2	1.75	Market Fuel
F	Summer Low	8.7	15.2	1.07	Fuel B + EtOH Splash-blend
G	Summer High	7.6	15.0	1.77	Fuel C + EtOH Splash-blend
H	Winter Low	14.2	15.3	0.64	Fuel D + EtOH Splash-blend
I	Winter High	13.3	15.3	1.61	Fuel E + EtOH Splash-blend
J	Summer High	8.7	0.0	2.48	Market Fuel
K	Winter Low	14.5	0.0	0.87	Market Fuel
L	Summer High	9.4	0.0	2.24	Fuel J + EtOH Splash-blend
M	Summer High	9.4	0.0	2.18	Fuel J + EtOH Splash-blend

Source: Table 1. *CRC Project RW-107-3: Validation of the New PM Index Formula.* Southwest Research Institute. April 2023.

3.2.2 Growth Energy 2018 Dataset

The Growth Energy dataset is the result of vehicle testing conducted at the UC Riverside CE-CERT laboratory during 2018 under the sponsorship of Growth Energy. The study investigated the effects of varying aromatics and ethanol levels on the exhaust emissions

of five GDI/SIDI vehicles. Two articles in the journal *Fuel* give results of the work: Yang 2019a on gaseous and toxic pollutants and Yang 2019b on particulate matter emissions. Table 3-3 summarizes the characteristics of the five SIDI vehicles in the test fleet. The MY 2016 and 2017 vehicles were certified to US EPA Tier 3 standards or to one of 3 corresponding California emission standards. Three are naturally-aspirated, while two are equipped with turbocharged air induction systems.

Table 3-3
Test Vehicles in the Growth Energy 2018 Study

PME Group	**SIDI (Tier 3 Certification)**				
	1	2	3	4	5
Model Year	2016	2017	2017	2017	2017
Engine Type	DI NA	DI NA	DI Turbo	DI NA	DI Turbo
Transmission	CVT	6-speed AT	6-speed AT	6-speed AT	6-speed AT
GDI Type	Wall-guided DI	Wall-guided DI	Wall-guided DI	Wall-guided DI	Spray-guided DI
Air Induction	Naturally Aspirated	Naturally Aspirated	Turbo-charged	Naturally Aspirated	Turbo-charged
EPA Cert	T3B30	T3	T3/B70	T3B70	T3B30
CA Cert	SULEV30 /PZEV	PC/PZEV	LEV3 /ULEV70	(none)	SULEV30 /PZEV
Source: Yang 2019a. *Table S1, Supplementary Material*					

The eight experimental gasolines are summarized in Table 3-4. The main experiment consists of five gasolines created by a specialty blender to cover 2 levels of total aromatics content (nominally 20 and 30 vol%) and three levels of ethanol content (0, 10, and 15 vol%). The Honda PMI index was determined after blending and was not directly controlled. The two low-aromatics gasolines have moderate to moderately-high levels for the Honda PMI (~1.75) while the three high-aromatics gasolines have high PMI levels (2.09-2.33). All five are of regular grade and a summer RVP of 9 psi. Added to these are three additional gasolines: a Tier 3 certification fuel with 10 vol% ethanol and two more gasolines created by splash-blending the Tier 3 gasoline to the E15 and E20 levels.

This dataset provides the opportunity to see, for the first time, the performance of PME in five Tier 3 SIDI vehicles at varying ethanol levels up to E15 and E20 (in one case). The CRC E-94-2 dataset (on which PME was based) contained only RVP 7 psi gasoline at E0 and E10 levels. The Growth Energy gasolines are a mixture of regular (87 AKI), intermediate (89 AKI), and premium grades (91.5 AKI with splash-blending). All have

RVP ~ 9 psi. This is a somewhat higher RVP level than the RVP ~ 7 psi of the E-94-2 gasolines on which PME was based, but RVP is not varied in the dataset. This dataset will test the predictive performance of PME on an independent set of gasolines and shed light on whether the designed linearity of PME with respect to Phase I PM emissions is retained in Tier 3 SIDI vehicles.

Table 3-4
Experimental Gasolines of the Growth Energy 2018 Study

	Match Blended					**Certification Fuel plus Ethanol Splash Blending**		
Property	Fuel 1	Fuel 2	Fuel 4	Fuel 6	Fuel 7	Fuel 3 Tier 3 Cert Fuel	Fuel 5 Fuel 3 -> E15 Splash	Fuel 8 Fuel 3 -> E20 Splash
Ethanol Content (vol%)	0.0	0.0	9.6	14.8	14.7	10.0	14.7	19.6
Total Aromatic Content (vol %)	21.2	29.4	29.1	21.8	29.3	21.4	20.3	19.1
Honda PMI	1.75	2.33	2.15	1.76	2.09	1.89	1.72	1.61
Octane Rating	88.1	87.2	87.0	88.6	87.4	87.8	89.8	91.5
RVP @ 100 F (psi)	8.9	8.8	9.2	9.1	9.1	9.0	8.8	8.6
Specific Gravity @ 60.0°F	0.742	0.754	0.757	0.751	0.760	0.746	0.748	0.751
Distillation 50% °C	100	113	97	70	73	87	71	72
Distillation 70% °C	126	141	137	124	133	126	124	120
Distillation 90% °C	160	172	169	163	170	159	158	155
Source: Yang 2019a. *Table 1. Physicochemical properties of the test fuels.*								

3.2.3 Due Diligence Assessment of the Emissions Datasets

Beginning with CRC Project E-94-2, a sequence of statistical tests and evaluations have been performed on new datasets to assure data quality before the statistical analysis was conducted. Assessments have included:

- Detection of outliers, if present. A statistical outlier is a data point that lies well away (either high or low) from most of the other values in a dataset such that it is an unlikely (but still possible) outcome of the experiment.

- Detection of drift in the calibration of laboratory instruments ("test cell" drift). The first and best line of defense against drift is always the attention given to instrument maintenance and calibration in the participating laboratories, but statistical tests for evidence of such drift were made as a precaution.

- Detection of emissions drift with vehicle odometer, which may occur due a variety of causes including normal aging, an undetected change in vehicle condition, etc.

- Repeatability of measurement, meaning the variability observed in repeated test runs for the same vehicle and gasoline.

The statistical methods used for these purposes in this project have been used in related statistical analyses since CRC Project E-94-2. They are identified and explained in Appendix H of the CRC E-94-2 report, which should be consulted by those interested in the specific methods and how they are applied.

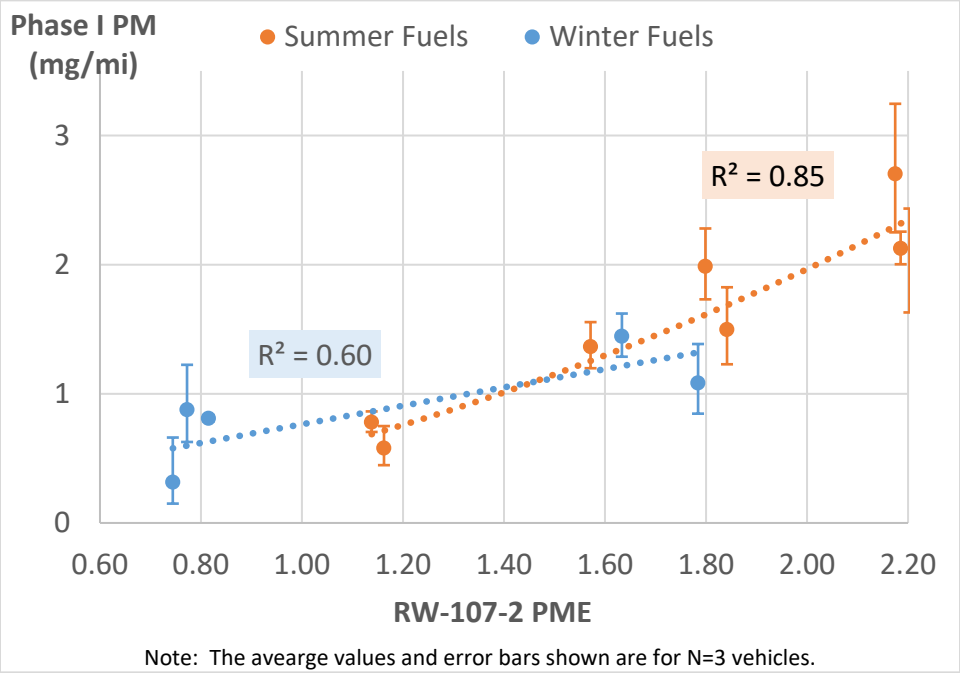
Both the SWRI and Growth Energy datasets passed the due diligence tests without concern. No cause was found to reject any of their data points as outliers, nor was evidence found of test cell drift or vehicle drift. The only quality difference detected between them was that the CE-CERT testing for Growth Energy had somewhat greater variability and lesser resolution for LA92 PM emissions. The resolution of Phase 1 PM measurement at the CE-CERT lab (Growth Energy 2018 study) was estimated as ~0.6 mg/mi compared to the estimate of ~0.25 mg/mi at the SwRI lab (CRC Project E-94-2). Although the testing was done at different laboratories under somewhat different testing protocols (such as the number of test runs conducted), both were found to be acceptable for use in this analysis.

3.3 PME Performance in the SWRI Dataset

The inclusion of summer and winter gasolines in the SWRI dataset gives the chance to investigate PME's performance across varying RVP levels. We begin with the group of three Tier 3 PFI vehicles, which is small as a test fleet but still capable of providing some insight to the performance of the vehicle type.

An early stage in the analysis suggested the possibility that the PM emissions response in PFI vehicles differed between the summer and winter gasoline groups in a manner not accounted for by PME. As indicated in Figure 3-1, the emissions slope for the winter gasolines (blue line) was found to be flatter than for the summer gasolines (orange line). However, the PM emission levels of these vehicles are very low and it was noted that gravimetric PM measurements are difficult to make below 1.0 mg/mi where the 3 lowest points lie. Thus, the reliability of the trend for winter gasolines was investigated.

Figure 3-1
PFI Vehicles: Phase I PM Emissions versus RW-107-2 PME
(Summer and Winter Gasolines)



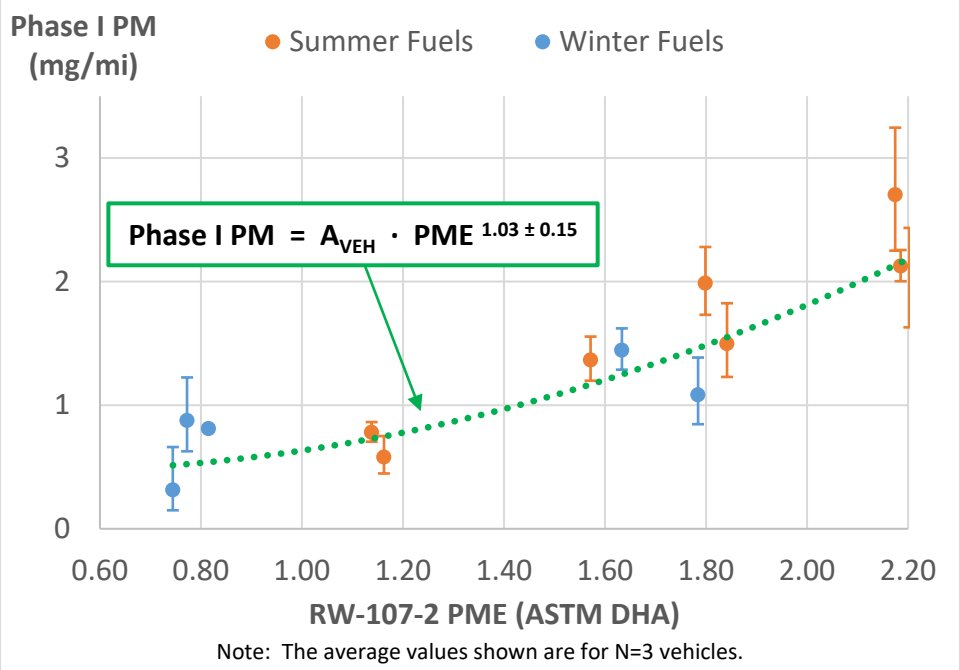
The resolution of Phase I PM measurements at the SwRI laboratory is ~0.25 mg/mi, which suggests that discrimination of PM values should be possible even below 1.0 mg/mi. MSS (micro soot sensor) measurements were examined to confirm this. MSS can be measured at very high resolution, but it represents only the soot (black carbon) component of PM and not the organic carbon components. Figures 4 and 5 in the SwRI testing report (see Appendix A) show that Phase I PM emissions are linearly related to MSS emissions over a very wide range with an intercept representing the missing PM components. Analysis of the MSS values for these vehicles on winter gasolines confirmed the trend seen in the figure and indicated that it was not an artifact of limited resolution at low emissions levels.

While the slope difference is statistically significant at the p=0.03 level, which many studies would report as statistically significant at the $p \leq 0.05$ level, this does not meet the $p \leq 0.01$ criterion for statistical significance that was adopted in CRC Project E-94-2 and used since. The two-slope model suggested by the figure also fails the F-test for reduction in error sum-of-squares compared to a model with just one slope. Thus, the final analysis concluded that PME performs well for indicating the Phase I PM emissions of PFI vehicles for both summer and winter gasolines and is applicable to gasolines spanning an RVP range of 7 to 15 psi.

The green line in Figure 3-2 is the best fit relationship of the log-form equation used to define PME: log(Ph 1Phase I PM) = A + B·PME. When exponentiated, it gives the boxed equation in the figure. With an intercept term allowed for each individual vehicle, the overall relationship shows PME to be directly proportional to Ph 1Phase I PM emissions in mg/mi. The exponential constant 1.03 ± 0.15 is indistinguishable from PME's design

value of 1.00, as a t-test for the observed difference from 1.00 readily confirms. Thus, the linearity of PME with PM emissions is found both in the fifteen Tier 2 PFI vehicles (from EPAct) on which PME was based and in the three Tier 3 PFI vehicles in the SWRI dataset.

Figure 3-2
PFI Vehicles: Relationship of RW-107-2 PME to Phase I PM Emissions



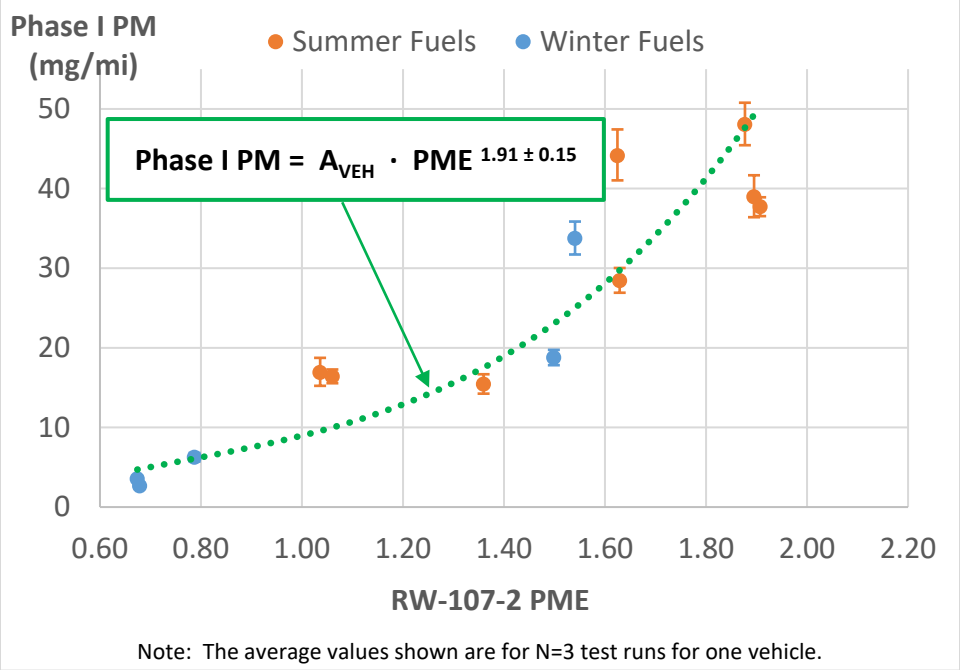
With regard to SIDI vehicles, little can be said based on the SWRI dataset because it contains only a single direct-injection vehicle. Any trend observed in the data pertains only to the individual vehicle and cannot be generalized to other SIDI vehicles as a group. For the SIDI vehicle, the dataset contains no evidence that summer vs. winter RVP differences influence Phase I PM emissions is a manner not accounted for by PME (see Figure 3-3).

For this vehicle, the direct proportionality between PME and Phase I PM emissions is broken. The best-fit (green) line indicates an exponential factor of 1.91 ± 0.15 rather than PME's design 1.00 value. Note that Vehicle B was provided by CRC and is one of the Tier 2 SIDI vehicles that participated in the E-94-2 and related testing. Thus, the higher exponent here is a vehicle-specific result within a 12-vehicle test fleet for which direct proportionality held overall. One must recognize that the PME versus Phase I PM proportionality will hold only for groups of vehicles and not necessarily for individual vehicles within the group.

3.4 PME Performance in the Growth Energy 2018 Dataset

The Growth Energy dataset gives a chance to investigate PME's performance in Tier 3 SIDI vehicles. The E-94-2 SIDI vehicles on which PME was based were all certified to Tier 2 standards. The five vehicles in Growth Energy were certified to reduced Tier 3

Figure 3-3
SIDI Vehicle B: Relationship of RW-107-2 PME to Phase I PM Emissions



standards and weighted-average LA92 PM emission levels (mg/mi) that are similar to the 6 lowest-emission vehicles of the twelve vehicles tested in CRC Project E-94-2 (which ranged up to nearly 50 mg/mi). Thus, the dataset can help answer whether the designed proportionality of PME and Phase I PM emissions (based on Tier 2 vehicles in E-94-2) continues to hold for Tier 3 SIDI vehicles.

The dataset also gives the chance to investigate PME's performance when gasolines are splash-blended from E10 to E15 and E20. In E-94-3, a subset of four vehicles was tested on E10 gasolines created by splash-blending E0 gasolines from E-94-2 to the E10 level for comparison with the match-blended E10 gasolines in E-94-2. There, it was found that PME under-estimated the Phase I PM emissions of splash-blended E10 gasolines.

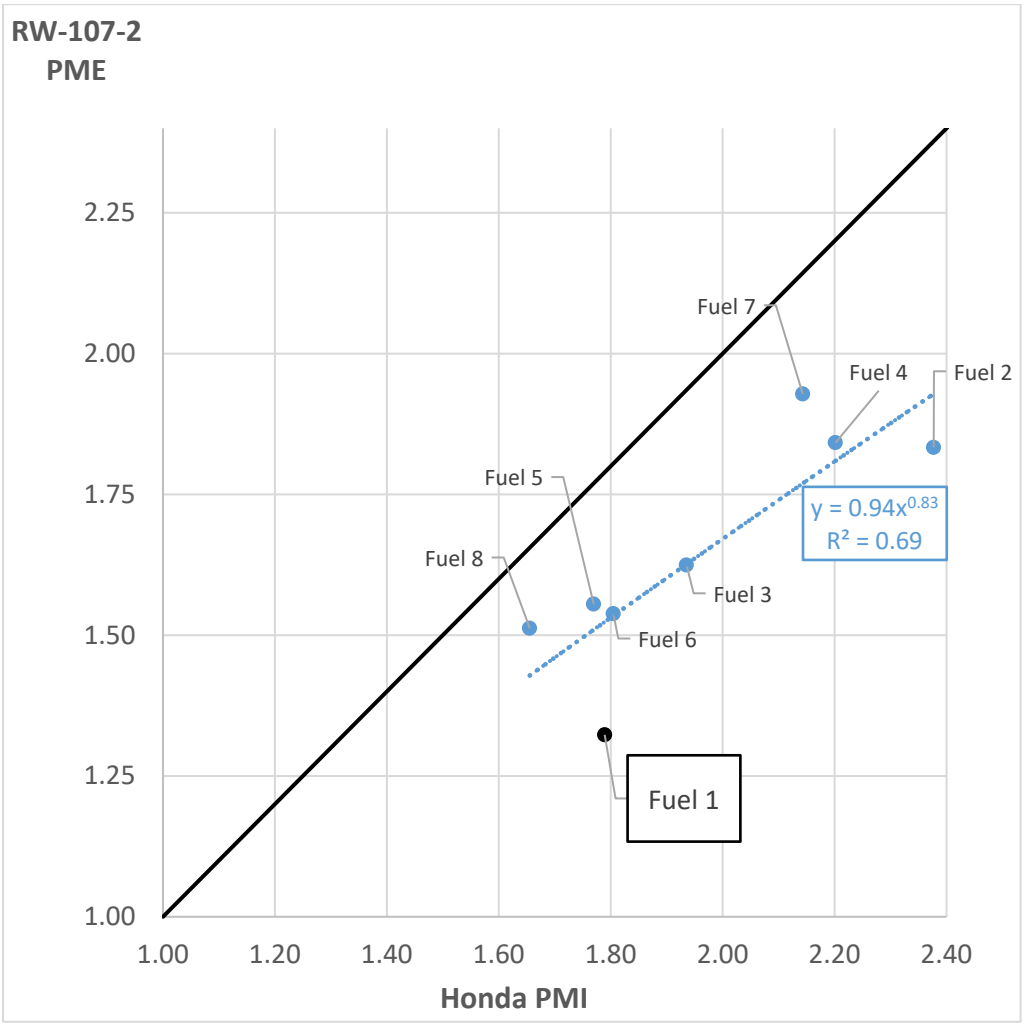
3.4.1 PME Performance Overall

With regard to the first question, analysis of the Growth Energy dataset quickly established that PME was a good indicator of Phase I PM emissions—except in the case of Fuel 1—but that the designed proportionality of PME and Phase I PM emissions was lost. Phase I PM emissions were found to increase at a faster-than-proportional rate as PME increased.

Figure 3-4 plots the PME index for the Growth Energy gasolines against their Honda PMI values. For the gasolines other than Fuel 1, the dotted trendline (blue) is typical of the relationship that is found between PME and PMI. In past studies, PMI has been found to increase more rapidly than Phase I PM emissions. Thus, when PME is linearized to be directly proportional to Phase PM, it must increase at a slower rate than PMI and fall

progressively further to the right of the (black) line of equality as seen in the figure. Fuel 1 (in black) lies significantly below the trendline by more than any other fuel.

Figure 3-4
RW-107-2 PME versus Honda PMI for Growth Energy Gasolines



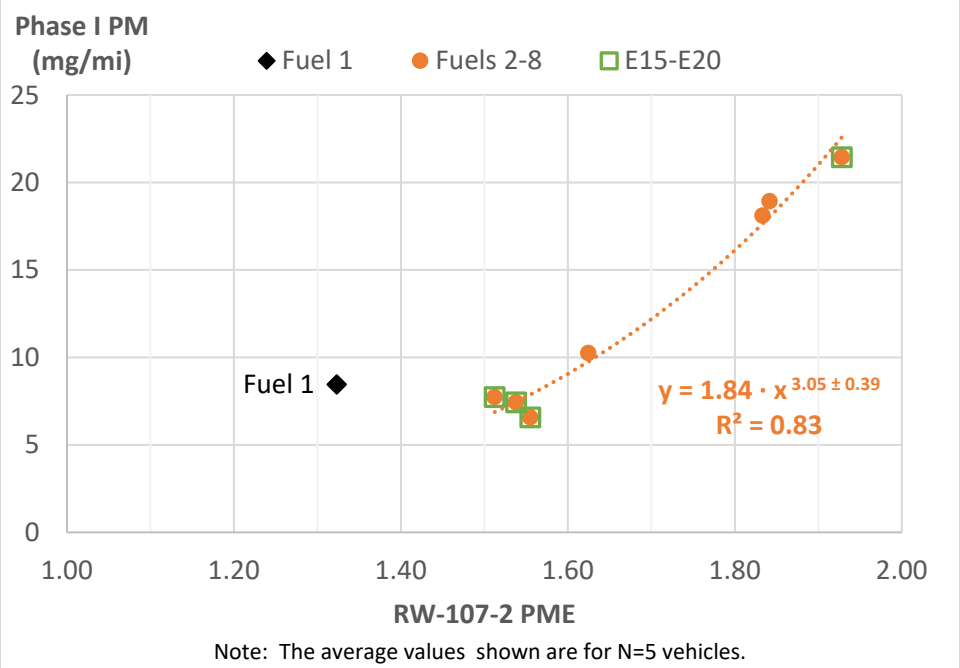
The Fuel 1 discrepancy becomes clearer when Phase I PM emissions are plotted against the PME (see Figure 3-5). All of the other fuels cluster closely around the orange trendline between Phase I PM and PME. Fuel 1 stands well to the left of the other fuels at its PME value of 1.32; in fact, its PME would need to be some 19% higher to place its average emissions data point on the orange trendline. Compared to the others, Fuel 1 was distinctive in having increased proportions of iso-paraffins and cyclo-paraffins (Napthenes) rather than n-paraffins in its low-aromatics blend. Further consideration of this is given in the next section.

For the other fuels, PME performs well as an indicator of Phase I PM emissions, accounting for 98% of the emissions variance among them. However, its empirical exponent is 3.05 ± 0.39, rather than the designed value of 1.00, so that the direct proportionality with Phase I PM emissions has been lost.

The implication of the larger exponent is that a 10% reduction in the PME value will translate into a 27% reduction in Phase I PM emissions of these Tier 3 vehicles, rather than the 10% reduction that would occur in Tier 2 vehicles. The larger percentage reduction would be taken off a lower base emissions level in Tier 3 vehicles, but would nevertheless be substantial in gm/mi terms. This is a conservative outcome in the sense that one can apply PME with confidence to estimate emission reductions from gasoline reformulation because the Phase I PM emission reductions for a mixed fleet of Tier 2 and Tier 3 vehicles will be as large or larger than the percentage reduction in the PME value itself.

Finally, PME is found to perform well for all four of the E15 and E20 gasolines, which are boxed in green in Figure 3-5. These include two splash-blended E15 and E20 gasolines created by adding ethanol to the E10 certification Fuel 3 and the two match-blended E15 and E20 fuels in the experiment on aromatics and ethanol content. This is the first time that PME for SIDI vehicles has been tested against an emissions dataset with gasolines having more than 10 vol% ethanol. Its success here validates the recommended extension of the α=f(EtOH) term beyond E10 at the same rate as its change from E0 to E10.

Figure 3-5
Growth Energy: Phase I PM Emissions versus the RW-107-2 PME



Note: The average values shown are for N=5 vehicles.

The RW-107-2 formulation of PME was based on a statistical representation of the sooting potential of hydrocarbon compounds called $yTerm_i$ that is proportional to YSI based on the 131 compounds in gasoline for which YSI had been measured. The $yTerm_i$ quantity was calculated from the molecule size (number of carbon and oxygen atoms minus one), the count of double bond equivalents outside of aromatic rings, and the number of aromatic rings in the molecule:

$$yTerm_i = (C+O-1) \cdot (1 + 1.7 \cdot DBE_{NON} + 5.6 \cdot ArRing_{FIRST} + 5.1 \cdot ArRings_{ADD}) \qquad (3\text{-}1)$$

As in the Honda PMI, saturated compounds are the reference point and given a value of 1 in the equation above. They are treated in PME as being uniform in sooting potential for a given molecule size (rather than uniform without regard to size as in PMI) and have the lowest propensity to form soot.

A concerted effort was made to determine how Fuel 1 differs from the other experimental fuels and to assure (through adoption of YSI) that the sooting potential of its chemistry was properly accounted for. Inquiries were made with the study sponsor to confirm that the PM emissions and DHA data received for Fuel 1 were those belonging to the original study. In the end, no explanation or hypothesis could be offered for the large apparent discrepancy between Fuel 1 and the others, leading to the decision to treat Fuel 1 separately from its counterparts in the analysis and graphs. It is not known whether the Fuel 1 discrepancy results from an unidentified fault in the underlying data or whether it is an indicator of a class of fuels for which PME (and possibly PMI) are not adequate indicators of PM emissions.

3.4.2 The Sooting Potential of Saturated Compounds

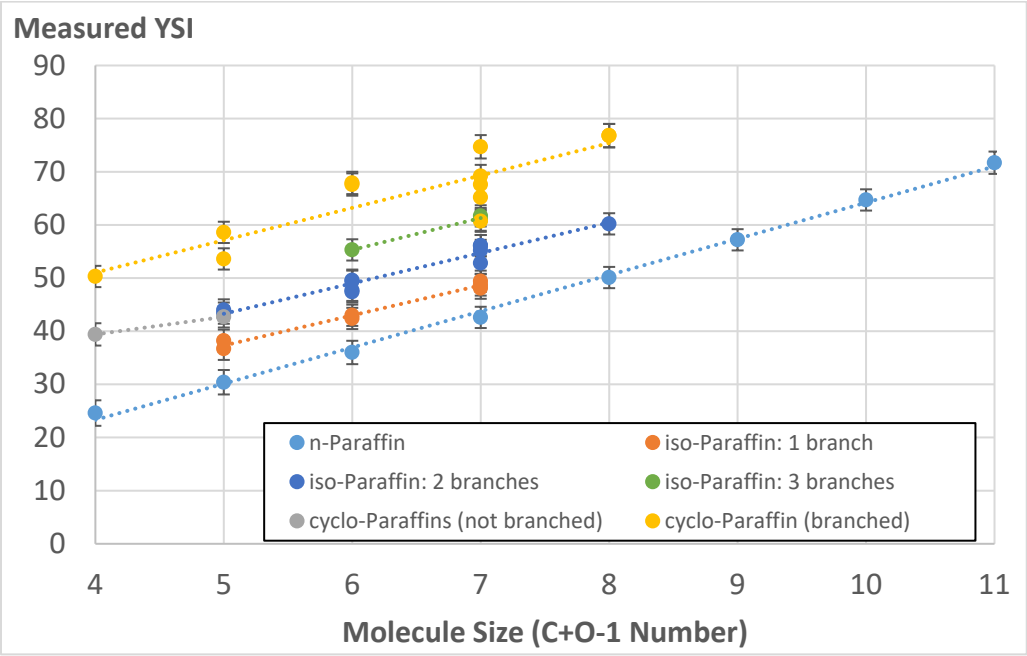
Investigation of the Fuel 3 discrepancy with its high fractions of iso- and cyclic-paraffins led to the discovery that the reality of soot formation in paraffins was more complex. As Figure 3-6 shows, both the type of saturate (whether n-, iso-, or cyclo-paraffin) and the number of branches in non-straight chain paraffins have an appreciable effect on sooting potential as measured by YSI. In some cases, these factors double the PM contribution of a compound. In the $yTerm_i$ formulation, the contribution of saturates would most closely follow the line for n-paraffins at the bottom. Thus, it will tend to undercount the sooting potential of gasolines like Fuel 1 with high fractions of branched and cyclic paraffins.

This discovery and the likelihood that branching also has an important effect in aromatic and olefinic compound groups led to the decision that $yTerm_i$ should be replaced by YSI values to improve the accuracy of PME across a broad range of gasolines. Other factors, such as the order in which molecules break down into radicals during combustion, may also influence sooting potential (St. John 2017) and will also be accounted for using YSI. Although motivated by the investigation of the Growth Energy Fuel 1, it will be seen later in this report that the adoption of YSI in PME did not resolve the observed discrepancy, which remains unexplained.

3.5 Summary

Table 3-5 presents a summary of what has been learned in the analysis on the validity and applicability of PME in Tier 2 and Tier 3 SIDI and PFI vehicles. PME is an effective and unbiased indicator of Phase I PM emissions for both SIDI and PFI vehicles certified to Tier

Figure 3-6
Effect of Type and Branching on Measured YSI of Saturates



2 or Tier 3 standards. It has been validated for use with E0 through E20 gasolines in both vehicle types and for gasolines with RVP ~ 7 to 9 in SIDI vehicles and 7 ~ 15 in PFI vehicles. For SIDI vehicles, it is likely that PME can be used with Winter gasoline as well, since no evidence has been found in this and the preceding project that RVP exerts an independent influence on PM emissions that is not accounted for by PME.

PME is directly proportional to Phase I PM emissions in 3 of the 4 groups so that a 10% reduction in PME translates to a 10% reduction in emissions. The proportionality is broken for Tier 3 SIDI vehicles in a manner such that a 10% PME reduction translates to a 27% reduction in emissions, although taken off a lower base level of emissions for Tier 3 vehicles.

It is reasonable to believe that PME's loss of proportionality and the increased exponent value is the result of changes in engine designs and controls that allowed these vehicles to meet the Tier 3 emission standards. A manufacturer wanting to reduce PM emissions in a SIDI vehicle would seek changes in design and controls to target the most common cause(s) for PM emissions formation. Such changes would then translate to reduced PM emissions for all gasolines, including ones with low and intermediate PM potential (whether measured by PMI or PME). However, the percentage reductions would be larger for low and intermediate gasolines PMI/PME and smaller for high PMI/PME gasolines where the inherent propensity of the gasoline to soot is of greater importance. Thus, sharpening of the PM emissions response to PME should be expected.

Table 3-5
Conclusions on Validity and Applicability of RW-107-2 PME

	SIDI Vehicles	**PFI Vehicles**
Development dataset	E-94-2 (12 Tier 2 vehicles)	EPAct (15 Tier 2 vehicles)
Validation dataset	Growth Energy 2018 (5 Tier 3 vehicles)	SWRI under RW-107-3 (3 Tier 3 vehicles)
Unbiased indicator of Phase I PM emissions?	Yes [a/]	Yes
Demonstrated Applicability	E0 through E20 RVP ~ 7 to 9 psi	E0 through E20 [b/] RVP ~ 7 through 15 [b/]
Directly Proportional to Phase I PM emissions:		
In Tier 2 vehicles?	Yes, by design	Yes, by design
In Tier 3 vehicles?	No. Exponent of 3.05 ± 0.39	Yes. Exponent of 1.03 ± 0.15

[a/] With the exception of Fuel 1.
[b/] EPAct established the PME range of validity for ethanol as E0 through E20 and for RVP as 7 to 10 psi.

4. REVISIONS TO THE PME FORMULATION

4.1 Introduction

While the RW-107-2 PME index proved to perform well as an indicator of Phase I PM emissions in the SWRI and Growth Energy datasets, the work also demonstrated that it could be improved. First, incorporating YSI in the numerator of PME in place of $yTerm_i$, its statistical representation, should improve the index's characterization of sooting potential for all individual hydrocarbon compounds. Second, and dating back to publication of the CRC Project RW-107-2 report, it had been recognized that PME's categorization of DHAs into "ASTM" and "SSI" groups was unsatisfactory, given that the real issue is the DHA's wt% coverage of the gasoline.

After consideration of the need, CRC decided to expand the scope of this project to include the work needed to revise and re-estimate the PME formulation. This chapter discusses the changes that were made. It concludes with a brief summary of how PME was re-estimated. Further information on the methodology for estimating PME can be found in Appendix B of the CRC Project RW-107-2 report.

4.2 Incorporation of YSI

A significant effort in this project was the work needed to organize the published DHAs into a consistent database. The database for RW-107-2 (used to develop PME) included DHAs done by SwRI and SSI for 70 gasolines from 6 different studies. Given the breadth of datasets, compounds, and data formats it became essential to compile a single unified database which included all compounds found in the experimental gasolines. This database was subsequently expanded to include all compounds within the current ASTM D6730-21 DHA standard and to add all properties necessary to calculate PME.

The diversity of data sources and formats, along with the number (1,182) of hydrocarbons that are found in the experimental gasolines, made this a daunting task. The DHAs were done over an extended period of time—from about 2010 for the EPAct DHAs to 2022 for the most recent SWRI data. While most were performed by SwRI, they are affected to some extent by differences over time in the master lists of compounds that are recognized in the DHA and in the inputs on boiling points and vapor pressures needed to calculate PMI and PME. Further, various formats were used to report and/or publish the DHAs. Quality control steps were imposed to assure accuracy; a key test was the ability to replicate (to within a small tolerance) the Honda PMI values reported for the gasolines in the original studies.

4.2.1 Other Property Assignments

The development of PME in RW-107-2 required several compound attributes to be added to the DHAs and SSI master list, including carbon count, single bond count, double bond count, ring count, and aromatic ring count. These counts were compiled manually.

Once it was decided that PME ought to include all compounds within the D6730-21 standard and it became necessary to add SMILES strings for YSI assignment, the PubChem API was utilized. This API allows one to automate the otherwise manual process of entering a compound name to return chemical data, such as molecular formula, molecular weight, SMILES, and IUPAC name from the PubChem database.

The automated API approach provided greater data quality as compared to manual compilation. The SMILES strings provided a convenient method for determining bond counts as well, which helped to check previous work. The IUPAC name output provided a standard naming convention across the entire database including those not found in the SSI Master database. PubChem outputs were compared against properties already present within the database such as molecular weight and DBE, along with a visual check of the compound names. This provided assurance that the PubChem API was accurately reporting molecular properties.

4.2.2 Generic Compound Standardization

The DHAs for gasolines include many compound entries which are only partially identified (so-called "generics"). One such compound is "C9_Mono-Naphthenes(4)". From the name it is clear that this compound has 9 carbons, 1 ring, and 0 double bonds (Naphtheno-Olefins are listed separately). Its molecular weight can be easily calculated and the double bond and ring count is sufficient to calculate a PMI value. However, this is not enough information to construct a SMILES string or estimate a YSI value.

A "representative" compound was assigned to each of these generic compounds and then used to obtain YSI and other information from PubChem. SSI used this approach in AVFL-29 to assign PMI values to generics. NREL also uses this approach in its work with the generics. Thus, the representative molecule approach was also adopted for the CRC database.

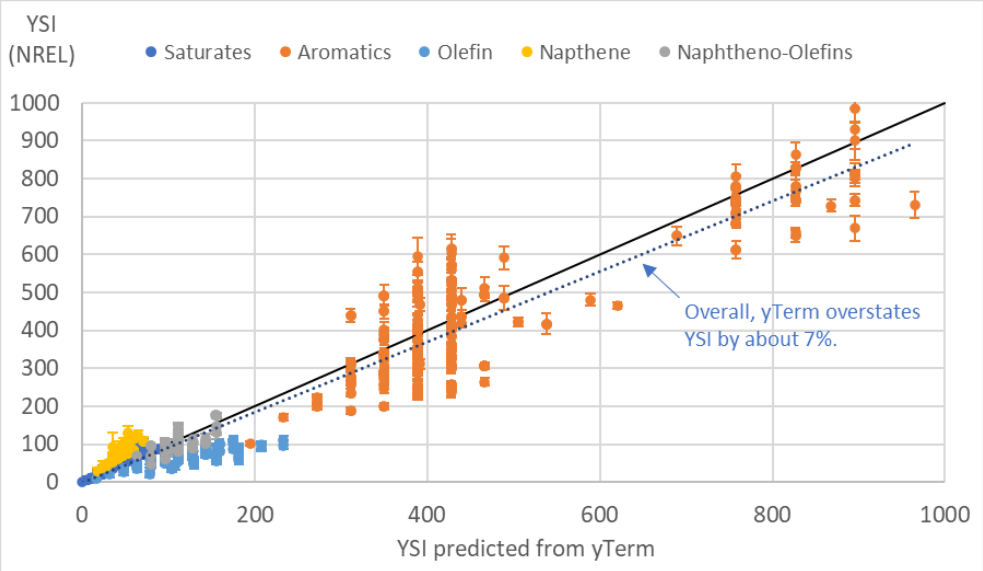
For the CRC database, generic compounds were assigned to the closest eluting compound based on the Retention Indices (RI) that shared the characteristics of the generic entry. The representative compound was then used to determine the YSI value. For the Honda PMI, the representative approach is not needed as the DBEs can be determined from the generic description. The representative molecule method used here would be highly likely to give the same result for PMI and could be verified. For purposes of estimating YSI through the online calculator, the representative molecule approach does not necessarily guarantee a correct value for the generics because no information is available on their branching. Without further description for the generics, a representative molecule based on RI was the best available approach.

4.2.3 Comparison to the yTerm$_i$ Representation

The incorporation of YSI was done to replace the earlier yTerm$_i$ representation of YSI that was used in RW-107-2 for the original PME index. As explained in Section 3.4.2, yTerm$_i$ was based on 131 compounds in gasoline for which YSI had been measured as statistical representation based on molecule size and counts of aromatic rings and the DBEs found outside of aromatic rings.

With all gasoline compounds assigned a measured or estimated YSI value, it becomes possible to assess the accuracy of the former yTerm$_i$ representation. Figure 4-1 compares YSI (measured and estimated) as provided by NREL to the YSI values that would be predicted from yTerm$_i$. All hydrocarbon compounds in the database are used in the figure, with large numbers of them overlapping below YSI~200. Only aromatic compounds are found above YSI~300. Overall, the yTerm$_i$ representation overstates YSI by about 7 percent (dotted blue line). This overstatement is corrected by the incorporation of YSI into the revised PME. Perhaps more importantly, the incorporation allows PME to capture the wide variation of sooting potential of individual compounds from the trendline and the group-specific trends for Saturates, Olefins, and Naphthenes at the low end of the graph. The incorporation of YSI is a significant improvement in the ability of the revised PME to accurately indicate sooting potential for a wide range of gasoline compositions.

Figure 4-1
Comparison of YSI to the YSI Predicted from yTerm$_i$



4.2.1 Standardization of Compound List and Vapor Pressures

In AVFL-29, SSI created an expanded list of compounds that can be identified in gasoline along with their DBE values, molecular weights, boiling points, and vapor pressures with the intent to improve identification of the heaviest compounds in gasoline. The SSI list of compounds has been adopted in the current D6730-21 DHA standard. This "SSI master"

list was utilized as a starting point for the database compound list, with additional compounds found in other DHAs added as necessary.

The values for vapor pressure ($VP_{443°K}$) in the SSI master list of compounds were adopted as the standardized values where available except for the oxygenated compounds for which empirical values were used. Empirical (measured) vapor pressures *must* be used for oxygenated compounds in gasoline because the correlation equation between VP_{443K} and BP given in Aikawa (2010) is valid *only* for non-oxygenated hydrocarbons. For compounds that did not exist in the SSI master list, boiling points and vapor pressures were taken from E-94, E-129, Growth Energy, and EPAct, in that order.

For oxygenates, VP_{443K} was standardized at the values reported by NIST as shown in Table 4-1 below. Note that i-Butanol and 2-methyl-1-propanol are equivalent compounds, although both appear in the SSI Master List with separate vapor pressures. Only i-Butanol is listed in Table X1.2 of ASTM D6730-21. These were standardized to a single boiling point value in this study. Users of PME are encouraged to adopt the standardized VP_{443K} for the oxygenates listed in the table below and to obtain and use empirical NIST values for other oxygenates found in gasoline.

Table 4-1
Vapor Pressure for Oxygenates in Gasoline (kPA at 443K)

Oxygenate	Standard Value NIST [a/]	SSI Master List	ASTM D6730-21 Table X1.2
Ethanol	1,475	853	854
i-Butanol	403	352	439
2-methyl-1-propanol	403	403	not listed
MTBE	1,075	1,075	1,436
[a/] https://webbook.nist.gov/			

While YSI has been measured for many compounds, empirical values are available for relatively few of the compounds found in gasoline. This made it necessary to use NREL's online YSI calculator[5] which estimates YSI based on compound structures entered as a SMILES string. Canonical SMILES strings, which represent bond configurations for each compound in the database,[6] were obtained using the PubChem API as discussed below. NREL assisted by running the full list of compounds through the website calculator to obtain the YSI values.

[5] See https://ysi.ml.nrel.gov/

[6] SMILES strings only represent bonds and do not differentiate stereoisomers such as "cis" and "trans" configurations, so the representations may not be unique for each compound named. The YSI prediction is the same irrespective of stereoisomer, so this is not an issue for this project.

4.3 Controlling for DHA Coverage in PME

The RW-107-2 PME recognized two classes of DHAs:

- An ASTM DHA procedure comparable to that performed by SwRI circa 2016-17 for CRC Project E-94-2 that identified 98 to 99 wt% of the gasolines by compound. Much earlier DHAs performed by SwRI for the EPAct project were also classified in the ASTM group although some achieved much lower coverage.

- The SSI DHA procedure that had recently been published in the CRC Project AVFL-29 report. This extension to the ASTM DHA procedure had been developed by SSI to extend the identification of compounds in gasoline to the level of 99.5 wt% or better. The SSI procedure has since been adopted in the current ASTM D6730-21 standard.

In reality, there are many different DHA procedures in use at laboratories, each of which is based on a version of the D6730 standard and with many having lab-specific extensions to the libraries used for peak identification. It is not possible to draw a class distinction between the various procedures in use.

In final review of the RW-107-2 report, a reviewer noted that the class distinction between DHA type should be replaced by a factor that expands the PME index based on the DHA's wt% coverage of the fuel. If 99 wt% of a gasoline was identified by compound in a DHA performed according to an early ASTM standard, a later DHA performed to the current D6730 standard that identified 99 wt% of a different gasoline should be equally complete. A method was needed to adjust the index value calculated from a DHA to constant coverage based on the wt% coverage of the underlying DHA.

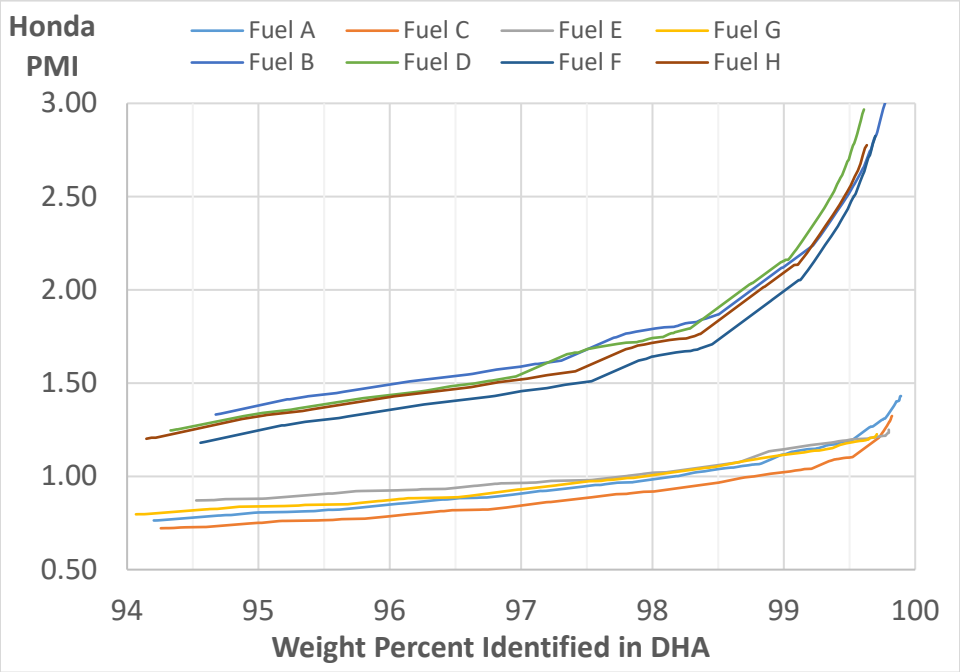
To address this need, the SSI DHAs for the E-94-2 experimental gasolines were examined to understand how the index value will change as the wt% coverage increases and to what extent the final index value (meaning at the maximum wt% coverage) can be estimated from an earlier index value at lower wt% coverage. The SSI DHAs achieved 99.5 to 99.9 wt% coverage for the eight E-94-2 gasolines and could be truncated at lower wt% coverages to simulate DHAs done with lower coverage.

A significant portion of a gasoline's PM potential is determined by heavy compounds eluting late in the DHA procedure. Figure 4-2 shows this for the E-94-2 gasolines by plotting the Honda PMI value that would be calculated as each new DHA peak elutes. As a group, the High PMI gasolines (top four lines) are clearly differentiated from Low PMI gasolines (bottom four lines) by the time that a total 95 wt% has eluted. The slopes of the curves (of PMI with respect to the wt% coverage) are also greater in the High PMI gasolines. Both groups have sharp upticks in the calculated PMI starting at about 98 wt% coverage for High PMI gasolines and about 99.5 wt% coverage for Low PMI gasolines. The extension of coverage to 99.5 wt% or better by the SSI procedure makes a large

contribution to understanding the PM formation potential of gasolines by identifying these peaks at the end of the elution curve.[7]

As the figure shows, DHA procedures can produce notably different PMI values for a given gasoline depending on their wt% coverage rates, particularly for High PMI gasolines. An early-version DHA that achieves only 95 wt% coverage would report a PMI of about 1.35 for an average High PMI gasoline, but would report values of about 1.75 with 98 wt% coverage, and about 2.50 with 99 wt% coverage. This range of values is wide enough to confuse the classification of a gasoline as being Low, Intermediate, or High in PM potential. Some means of standardizing the PM index for DHA coverage is required.

Figure 4-2
Dependence of Honda PMI Value on Wt% Coverage by DHA



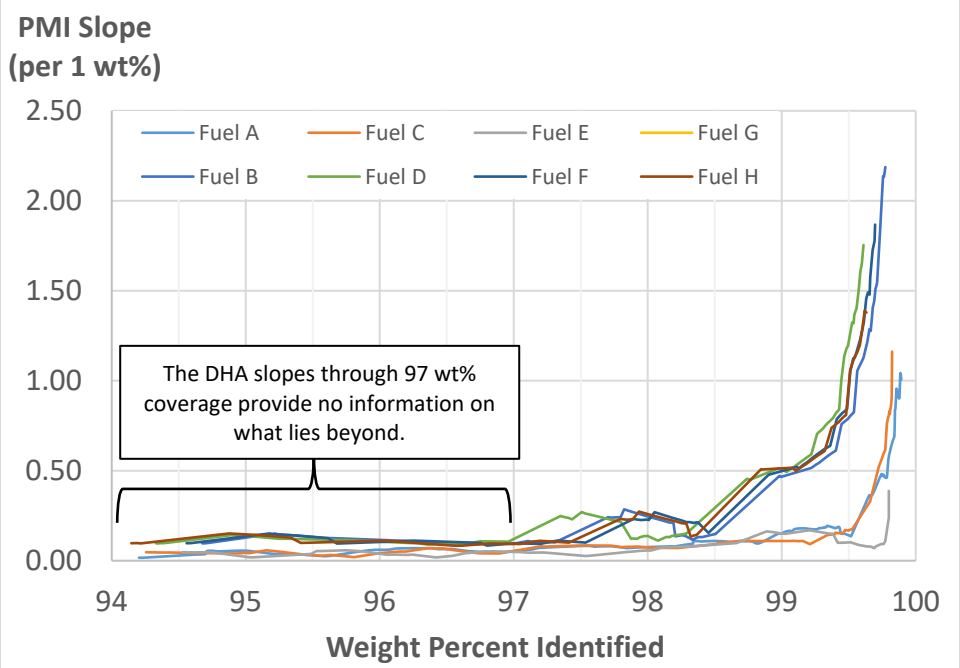
An effort was made using the E-94-2 gasolines to predict the PMI value at the end of the SSI DHA as a function of the wt% coverage and PMI value and slope of the PMI curve at varying points on the DHA. The local slope of the DHA was chosen as a factor that might tailor the expansion of calculated PMI values to characteristics of the individual gasoline. However, this effort was unsuccessful as the best models had, at best, only modest predictive power for the endpoint PMI values of the gasolines, which came at the expense of considerable complexity.

One reason for this is that the DHA slopes through 97 wt% coverage do very little to distinguish Low and High PMI gasolines and they provide essentially no information on the trend in DHA slopes and PMI values as the coverage increases (see Figure 4-3). It is

[7] Although unidentified peaks can occur at any elution time in the DHA, it is the unidentified peaks at the end of the DHA that have disproportionate impact on a fuel's PM potential and that were characterized in the SSI DHA procedure developed under CRC AVFL-29.

not until nearly 98 wt% coverage that High PMI gasolines diverge from Low PMI gasolines and not until 99 wt% and higher that the final upticks in PMI arise. A key conclusion is that it is not possible to adequately characterize the PM formation potential of gasolines using DHAs that provide 97 wt% coverage or less. A 98 wt% coverage is the minimum needed in a DHA and 99 wt% or higher is preferred.

Figure 4-3
Slope of PMI Curves as a Function of Wt% Coverage



Without success in modeling the expansion of PMEs from low-coverage DHAs to estimate high-coverage equivalents, a simplified approach was taken to this problem. First, a decision was made to exclude gasolines for which the DHAs provided appreciably less than 98 wt% coverage. This resulted in dropping 9 of the 27 EPAct gasolines, for which the DHA coverage ranged from 94 to 97 wt%, from the estimation of PME for PFI vehicles. These gasolines are believed to have been blended and tested at an early stage of the multi-phase EPAct work. The remaining gasolines have DHA coverage rates comparable to those of the E-94-2 gasolines done at the SwRI laboratory circa 2016-17.

Second, a decision was made to adopt 99.9 wt% as the reference point to which the revised PME values are expanded. This value is this highest of the coverage rates achieved by the SSI DHAs for the E-94-2 gasolines, which ranged from 99.6 to 99.9 wt%. This places the reference point at a level that can be achieved by the best current procedure.

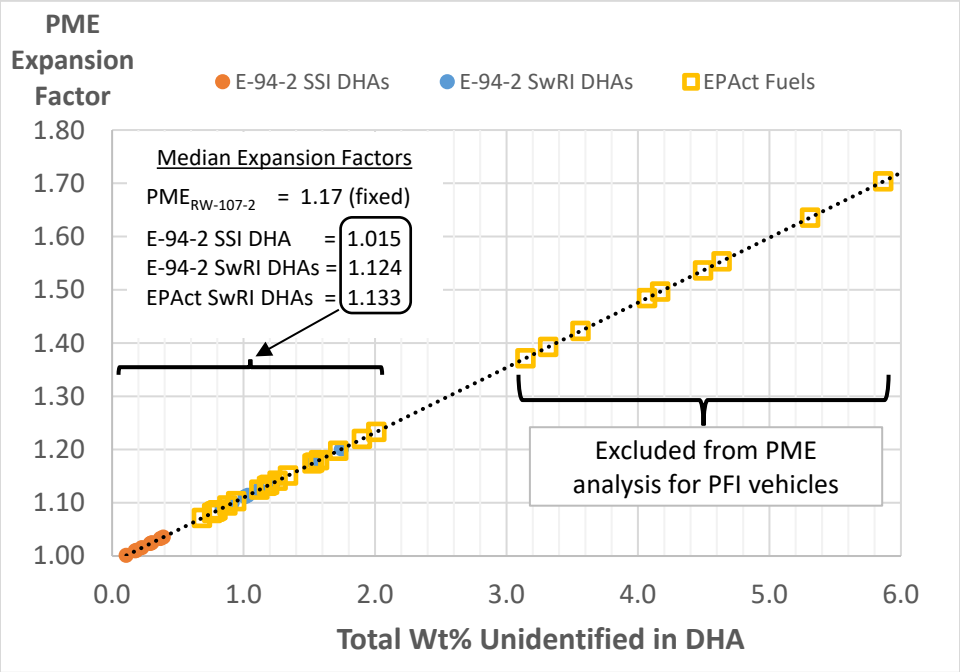
The PME expansion factor β was estimated along with the other empirical coefficients in the analysis of the E-94-2 data where both ASTM and SSI DHAs were available for each gasoline. The mathematical form of the adjustment was:

$$PME_{99.9} = PME_{EOC}^{\,(1 + 0.122 \cdot UnID)} \qquad (4\text{-}1)$$

where PME_{EOC} is the revised PME value calculated from the DHA (at the end of its curve) and UnID is the total wt% that remained unidentified by compound in the DHA. The resulting β value was determined to be 0.122 per 1 wt% coverage loss.

As Figure 4-4 shows, when this value is applied to the datasets used in estimating the New PME, the median expansion factors are 1.12 and 1.13 for the E-94-2 and EPAct datasets using SwRI DHAs and only 1.015 for the SSI DHAs. For the SwRI DHAs, the expansion factors range from 1.08 to 1.23 compared to the fixed 1.17 expansion adopted in the original PME. The necessity of excluding some low-coverage EPAct gasolines is demonstrated by the very high expansion factors they would otherwise require.

Figure 4-4
New PME Expansion Factor β for E-94-2 and EPAct Gasolines



4.4 Scaling of PME to Honda PMI

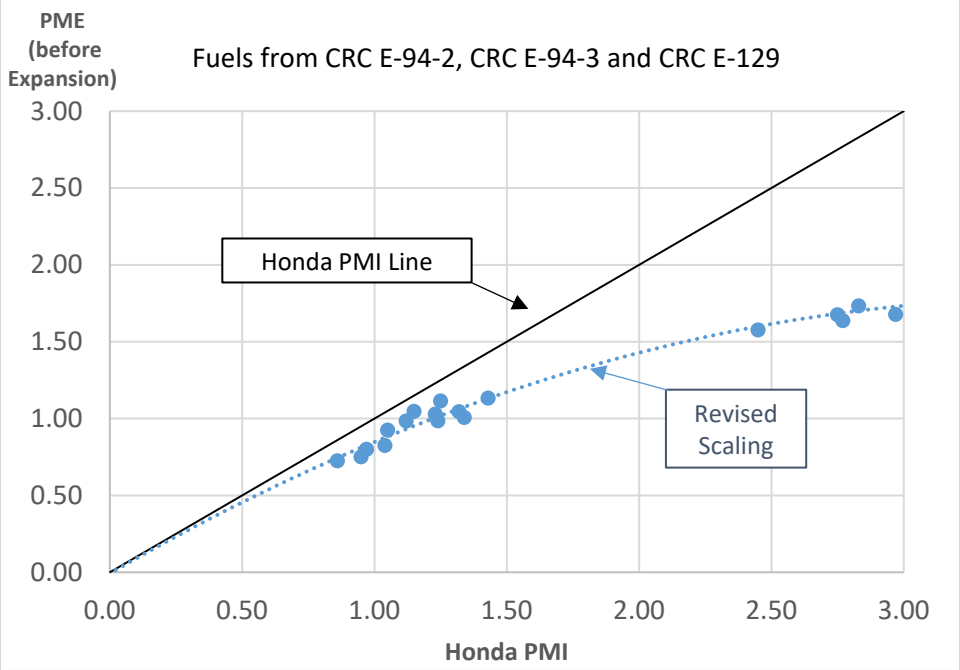
A final revision was made to the methodology for determining PME. The "raw" PME value computed from the summation term in Eq. 1-2 can be as high as 100 to 1000. Some form of scaling is needed so that PME can be compared intuitively to Honda PMI values. This implies that the PME value should be close to 1.00 for a gasoline that evaluates to a Honda PMI of 1.00.

In the RW-107-2 PME, scaling was accomplished by fitting a straight line to the plot of raw PME values versus Honda PMI and computing the implied raw value at PMI = 1.00. This value was used as a divisor to scale the raw PME values down to produce an expected value of PME = 1.00 for a gasoline with PMI = 1.00. This scaling, which is not apparent to the PME user, has worked satisfactorily thus far, but it rests on a false assumption regarding the relationship between PME and PMI.

Past studies of PM emissions, including CRC Project RW-107 and CRC Project RW-107-2, have shown that Phase I PM emissions do not increase as rapidly as the Honda PMI index would imply. PME corrects this problem so that Phase I PM emissions and PME are directly proportional. PME and PMI must both be zero at the hypothetical origin (a non-sooting gasoline), but PME must increase more slowly than PMI as the sooting potential increases. This means that PME must be somewhat less than 1.00 for a gasoline with PMI = 1.00 and that the gap between PMI and PME should widen as the sooting potential increases.

Figure 4-5 uses the gasolines from CRC Projects E-94-2, E-94-3 and E-129 to illustrate the relationship that is the basis for the new method of scaling. The New PME values shown are before scaling for DHA coverage. The N_{TECH} coefficient in New PME is the empirical scaling coefficient that results from the scaling with respect to Honda PMI.

Figure 4-5
Revised Scaling of New PME with respect to Honda PMI



4.5 Re-estimating Coefficients of the New PME

The other empirical coefficients of PME are estimated using a multistage, iterative process. The process begins with the SIDI vehicles, for which both ASTM and SSI DHAs are available for each gasoline to estimate the expansion factor coefficient β. The objective of the fit is to find the set of coefficients {α_{E0}, α_{E10}, and β} such that 3 conditions are met simultaneously:

- PME is found to be directly proportional to Phase I PM emissions in the group of E0 gasolines from CRC Project E-94-2.

- PME is also found to be directly proportional to Phase I PM emissions in the group of E10 gasolines in CRC Project E-94-2.
- Both conditions remain true when using either ASTM or SSI DHAs after their expansion to 99.9 wt% equivalents.

Three coefficients can be uniquely determined to meet three independent conditions applied to a set of data. Familiar regression methods such as ordinary least squares and non-linear least squares cannot perform the fit because their objective functions cannot accommodate the three-part condition in this problem.

Instead, an iterative method was used to search the parameter space of coefficient values to find the set that fulfills all three conditions. Given a starting pair of $\{\alpha_{E0}, \alpha_{E10}\}$ values, the β coefficient was varied until the expanded PME values from ASTM and SSI DHAs were equivalent, meaning that the ASTM $PME_{99.9}$ equals the SSI $PME_{99.9}$ with minimum error. At that point, a grid search was performed around the starting $\{\alpha_{E0}, \alpha_{E10}\}$ values to find the values that fulfilled the two proportionality conditions with minimum error given the β value just determined. The process was then repeated to re-estimate β and $\{\alpha_{E0}, \alpha_{E10}\}$ until changes in the coefficients were on the order of 0.003 or smaller. This determines the empirical coefficients for the PME equation for SIDI vehicles.

For PFI vehicles, the β value determined for SIDI vehicles was applied to the reduced EPAct dataset of 18 gasolines. A comparable iterative search was then conducted for the set of coefficients $\{\alpha_{E0}, \alpha_{E10}$, and $\alpha_{E20}\}$. Because the number of E15 gasolines is small, the α coefficient for E15 is assumed to lie halfway between α_{E10} and α_{E20}. Thus, three coefficients are fit in an iterative fashion until changes in the coefficients were on the order of 0.003 or smaller. This determines the empirical coefficients for PFI vehicles.

4.6 PM Emissions Datasets Used to Re-estimate PME

In RW-107-2, PME was developed using the E-94-2 fuels and PM emissions data for SIDI vehicles and the EPAct fuels and PM emissions data for PFI vehicles. This choice gave balanced datasets of 12 and 15 vehicles in which each vehicle was tested on 8 and 27 gasolines, respectively. Balanced design is highly desirable because it assures that coefficient values estimated from an analysis are not biased by uneven coverage, as can happen when one or more experimental fuels are tested in some vehicles but not in others. Smaller emission datasets from the CRC E-94-3 and E-129 studies were excluded from the PME development because their inclusion would break the balanced design.

All of the vehicles in the E-94-2 and EPAct datasets were certified to Tier 2 emission standards for PM, making the PME index homogeneous and specific to the technology level used in achieving the Tier 2 PM standards. The Tier 3 PM standards required reductions in PM emissions from SIDI vehicles but placed little or no pressure for emission reductions on PFI vehicles. Changes in certification standards and vehicle technology have the real potential to change the relationship between PME (or any other PM index) and the Phase I PM emissions of vehicles.

New decisions were required on which datasets to include in the re-estimation of the PME index in this work. The Growth Energy dataset of 5 SIDI vehicles and the RW-107-3 dataset of 1 SIDI and 3 PFI vehicles were the only new, independent datasets on PM emissions from vehicles that had been published since the E-94-2 and related studies. While small in terms of their vehicle fleet sizes, they are suitable for independent testing of PME performance, as reported in Section 3. Whether they should be included in the dataset used to re-estimate PME is another matter. Ultimately, a decision was made to exclude them and base the re-estimation on the E-94-2 dataset for SIDI and the Reduced EPAct dataset for PFI, much as in the prior RW-107-2 study.

Several reasons motivated this decision. First, their inclusion would break the balanced nature of the main datasets and introduce statistical complications. Given the small number of additional vehicles and fuels, the gain from expanding the dataset was judged not enough to offset the added complications. Second, their inclusion would introduce effects caused by emission differences between Tier 2 and Tier 3 vehicle technologies, because all of the Growth Energy vehicles were certified to Tier 3 standards as were 3 of the 4 RW-107-3 vehicles. The likelihood of a differential emissions response for Tier 3 vehicles (at least for SIDI) was large enough that the datasets should not be pooled, but the dataset sizes were not large enough to permit the reliable estimation of PME parameters specific to Tier 3 vehicles.

Further, for SIDI vehicles, the Growth Energy study (the sole source of data for Tier 3 SIDI vehicles) was conducted at a different laboratory than the others. While the data were evaluated and found to be of good quality, this situation necessarily confounds the differential performance of PME in Tier 2 and Tier 3 vehicles with any lab-to-lab differences that might be present. It is not possible to disentangle the two.

Given these considerations, it was judged best to re-estimate PME using the CRC E-94-2 and the Reduced EPAct datasets of Tier 2 vehicles so that the New PME is homogenous and specific to Tier 2 vehicle technology as before. Then, the performance of New PME on the Growth Energy and RW-107-2 datasets can be used to comment, to the extent the data permit, on how Tier 3 and later technologies might differ in terms of their emissions response to fuels. The latter has been done and is reported in Tables 3-5 and 5-3.

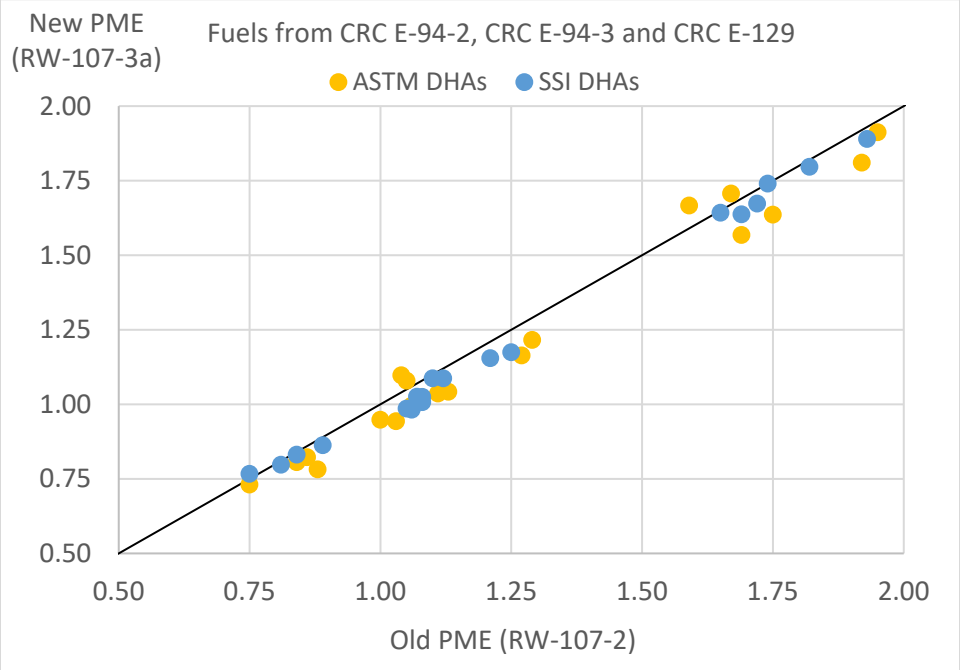
4.7 Comparison of Old and New PME Values

Section 5 of this report presents the performance of the New PME index for indicating Phase I PM emissions from SIDI and PFI vehicles. As a prelude to that, this subsection presents a simple comparison of Old and New PME values as calculated, respectively, from the original PME formulation (CRC RW-107-2) and the revised PME formulation developed here.

As Figure 4-6 makes clear, there is very little difference between Old and New PME index values when evaluated for SIDI vehicles using the fuels of the three CRC emission studies. Similar values are obtained whether the index values are computed from ASTM or SSI DHAs with their differing wt% coverage of fuel composition. New PME changes the form of the expansion factor to be a function of the DHA wt% coverage, while the expansion

factor for Old PME was a fixed gross-up of about 17% (β=1.17) for ASTM DHAs. The similarity of old and new values reflects that the underlying dataset for SIDI vehicles is unchanged and the form and coefficients of PME are very similar.

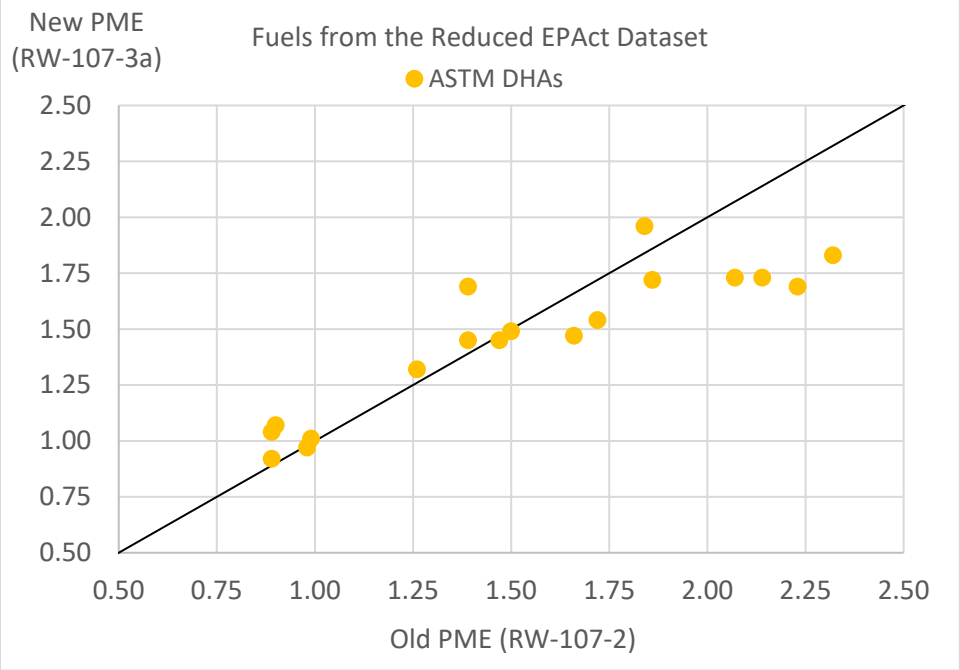
Figure 4-6
Comparison of Old PME and New PME Values for SIDI Vehicles



For PFI vehicles, Figure 4-7 shows that there is good overall correspondence between Old and New PME values for fuels in the Reduced EPAct dataset, but there is a greater degree of scatter and some systematic difference for Old PME values above 2.00. Here, the underlying dataset was changed by removing one-third of its fuels with wt% coverages below 98 wt% in their ASTM DHAs (no SSI DHAs exist). For Old PME, these fuels shared the same ~17% expansion of the calculated index value as the other EPAct fuels, but for New PME would require expansion factors of +30% or more (see Figure 4-4).

The reduced wt% coverage of the excluded fuels means that their DHAs carry little useful information about the PM potential of the fuels (see Section 4.3 and its Figure 4-3). By excluding them in the estimation of New PME, the coefficients for PFI vehicles are changed substantially. This, along with the other methodological and data changes, causes New PME to give substantially different evaluations of the PM potential of fuels than before, which introduces the scatter. One fuel with Old PME of about 1.80 is now ranked the highest of all with a New PME of nearly 2.00. The group of four fuels with Old PME values ranging from 2.05 to 2.30 are now lower ranked at a New PME value of about 1.75. It is not a surprise that the largest differences occur at high index values, as the issues surrounding wt% coverage (the exclusion of fuels and expansion for wt% coverage) are primarily related to the late-eluting compounds in the DHA procedure that have disproportionate impact on a fuel's PM potential. New PME should be a more reliable indicator of the relationship between fuel composition and Phase I PM emissions.

Figure 4-7
Comparison of Old PME and New PME Values for PFI Vehicles



5. THE NEW PME FORMULATION

5.1 The New PME Formulation

The New PME formulation is presented in Figure 5-1. It is intended as a replacement for the PME developed in CRC Project RW-107-2, which is now obsolete and should not be used. Where necessary to avoid confusion, the New PME can be written as $PME_{99.9}$ to denote the expansion of the index value to the reference 99.9 wt% coverage.

Figure 5-1
The New PME Formulation

Direct Proportionality (1.0)

$$\text{LA92 Phase 1 PM} = A_{Veh} \cdot PME_{Eng\ Tech}^{1.0}$$

Empirical parameters are in orange.

$$PME = \left(\frac{43.4}{LHV}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot YSI_i}{VP_i^{\alpha=f(EtOH)}} \right]^{(1+\beta\cdot(99.9-FuelCoverage_{DHA}))}$$

$$\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$$

$$f(EtOH) = \alpha_{E0} + \Delta\alpha \cdot EtOH_{VOL\%}$$

$FuelCoverage_{DHA}$ = Total Wt% Identified in DHA

LHV = Lower Heating Value

Engine Technology	DHA Type	N_{TECH}	α_{E0}	α_{E10}	α_{E15}	α_{E20}	β
SIDI	ANY	0.001025	0.451	0.430	0.419[a/]	0.409 [a/]	0.122
PFI	ANY	0.000558	0.257	0.250	0.236	0.222	0.122

[a/] Recommended extension to E15 and E20 based on the α_{E0} to α_{E10} trend.

As seen in the figure, the New PME is based on a definitional equation that requires the LA92 Phase I PM emissions of a group to vehicles to be directly proportional to the PME index. Given this, a 10% reduction in the index will correspond to a 10% reduction in Phase I PM emissions. The direct proportionality is indicated by exponential value of 1.00

that is circled in the figure. Based on the analysis in this section, it applies to Tier 2 PFI and SIDI vehicles and to the Tier 3 PFI vehicles in the SWRI dataset. The proportionality is broken for the Tier 3 SIDI vehicles in the Growth Energy dataset, most likely as a result of engine changes needed to certify to the lower Tier 3 PM standards.

The formulation is built around a modification to the Honda PMI Equation. The summation term in PME is calculated across the hydrocarbon compounds identified in a DHA. The numerator contains the YSI_i value for compound *i* as the indicator of its sooting potential, rather than the $1+DBE_i$ term of the Honda PMI or the $yTerm_i$ value of the Old PME. The YSI values include both measured values and values estimated from the NREL online YSI calculator. The values cover <u>all</u> of the compound identifications in Table X1.2 of the ASTM D6730-21 DHA standard plus the additional compounds that have been found in DHAs performed (according to earlier versions of the standard) for experimental gasolines of the EPAct, CRC E-94-2, E-94-3, and E-129 studies.

The denominator of the summation term is a generalization of the inverse vapor pressure (1/VP) term in the Honda PMI to the form $1/VP^{\alpha}$. The α term depends on the engine technology (PFI or SIDI) and is a linear function of the ethanol content of the gasoline. The α exponent adjusts the relative contributions to sooting potential of the individual compounds to account for the fact that differential vaporization of the compounds modifies the bulk fuel composition by the time that combustion of fuel droplets begins.

Once the summation term is fully evaluated, it is scaled by an empirical coefficient N_{TECH} so that PME values will be of the same order of magnitude as PMI and can be intuitively compared. The method of scaling was described in Section 4.4.

The scaled PME value resulting from the summation will be numerically larger or smaller for any given gasoline depending the total wt% that was identified by compound in the DHA. The New PME formulation standardizes the scaled PME values for DHA coverage to a reference level of 99.9 wt%, which is the highest value reached in any of the experimental gasolines using the SSI DHA procedure. The same coefficient $\beta = 0.122$ is used for PFI and SIDI vehicles to calculate the expansion factor term given in the figure.

Finally, the expanded PME value is adjusted for the energy content of the gasoline (LHV). Gasolines vary somewhat in energy content depending on composition but, more importantly, their energy content per kilogram (kg) or gallon is reduced by the addition of ethanol or other oxygenates that have lower energy content per wt% or vol%. Everything else being the same, more kg's of E10 gasoline will be required to power a vehicle over the LA92 driving cycle than if an E0 (ethanol-free) gasoline were used. As the summation term of PME has units of soot formed per unit mass, PME is scaled for energy-content using 43.4 MJ/kg as a standard value for ethanol-free reformulated gasoline (GREET 2019).

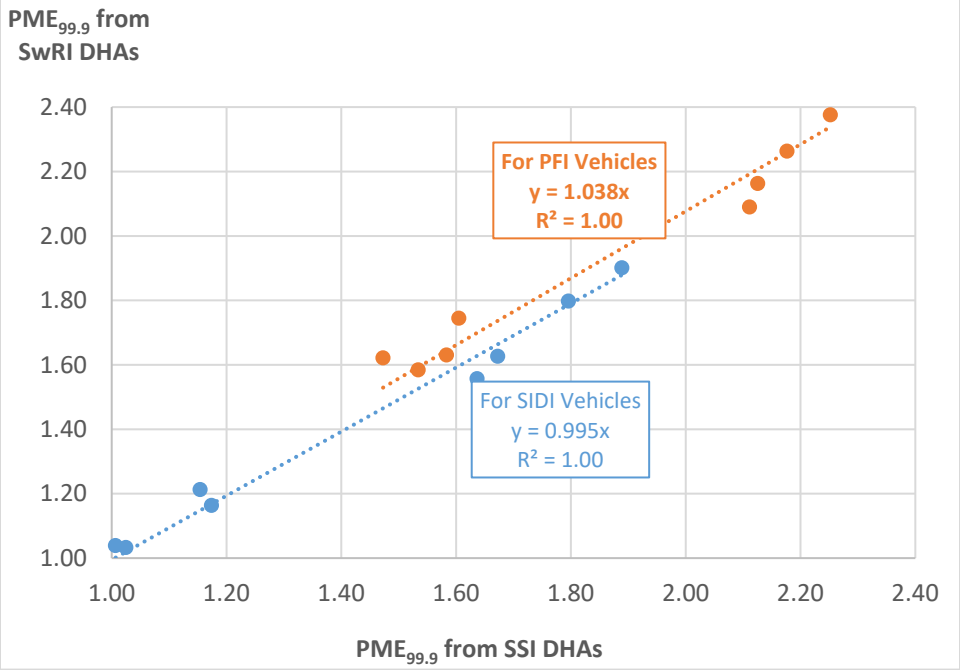
As given in the lower portion of the figure, two sets of empirical coefficients are given for New PME. One set pertains to SIDI vehicles and the other to PFI vehicles. A spreadsheet-based PME calculator is available from CRC that will translate a DHA into two PME index

values—one for PFI and another for SIDI. The E-94-2 dataset on which the SIDI coefficients are based does not contain gasolines above E10. The Growth Energy dataset demonstrated that the E0 to E10 trend can and should be extended to E20 as footnoted in the figure. The EPAct dataset on which the PFI coefficients are based contains gasolines through the E15 and E20 levels.

As explained at the end of Section 4, the β coefficient was derived in the estimation of New PME for SIDI vehicles by requiring that the direct proportionality conditions apply both for the "ASTM" DHAs done by SwRI and the corresponding SSI DHAs once their PME values are expanded to be 99.9 wt% equivalents. This condition implies that the expanded ASTM and SSI PME values should be the same or nearly the same.

Figure 5-2 demonstrates the equivalence of the expanded PMEs using the eight E-94-2 gasolines. The blue points and line represent the results for SIDI vehicles, taken from the PME estimation for SIDI vehicles. There, the expanded SwRI DHAs yield PMEs that are 0.5 percent lower on average than the PMEs from the expanded SSI DHAs. The 1-sigma range for individual gasolines is ± 4.3 percent around the blue trendline. The orange points and line show the results for PFI vehicles, once the PME model for PFI vehicles is applied to the E-94-2 gasolines. There, the expanded SwRI PMEs average 3.8 percent higher than the SSI PMEs, with a 1-sigma range of ±6.4 percent among gasolines. This correspondence is judged to be satisfactory for purposes of a PM index.

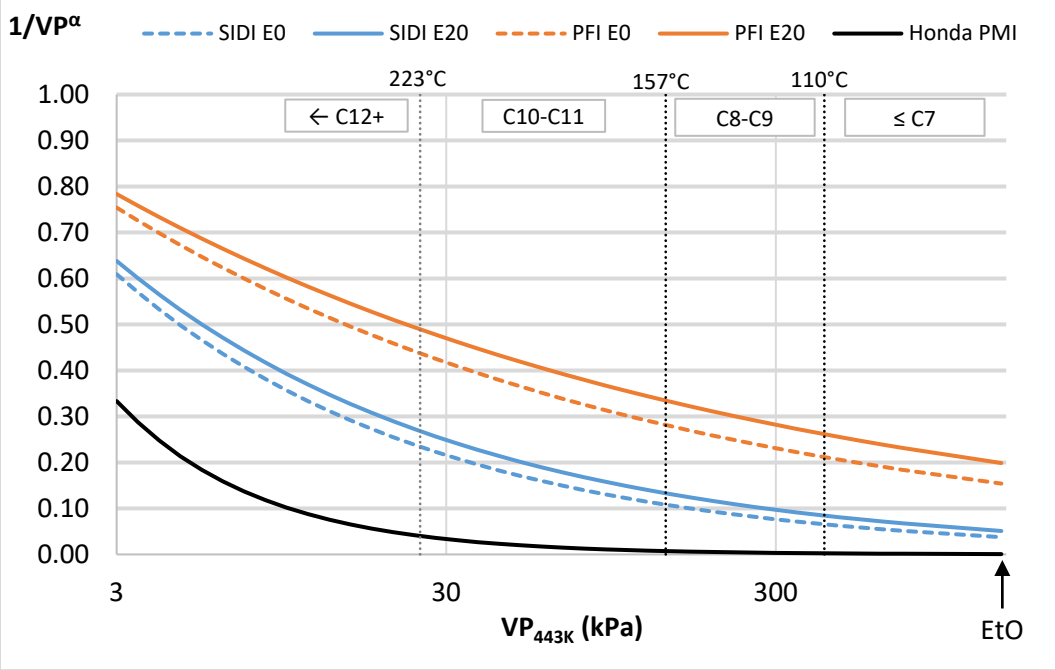
Figure 5-2
Equivalence of Expanded New PMEs from SSI and SwRI DHAs



The set of α coefficients for New PME govern the relative contributions of the individual compounds to soot formation at the time that combustion takes place, depending on engine technology and the ethanol content of the gasoline. Figure 5-3 shows curves for the relative

contribution to soot formation as a function of vapor pressure. The curve for Honda PMI is shown at the bottom in black. Its 1/VP term indicates that only the heavy, low vapor pressure compounds in the C10 and higher range make large contributions to soot formation. The New PME for SIDI vehicles is shown in blue for E0 and E20 gasolines and for PFI vehicles in orange for E0 and E20 gasolines. For SIDI vehicles, the $1/VP^{\alpha}$ term says that heavy compounds make about 12 times the contribution to soot as the light compounds (a 0.60 value at 3 kPa versus .05 value at the vapor pressure for EtOH) at the time combustion takes place. For PFI vehicles, heavy compounds make about 5 times the contribution of light compounds (0.75 at 3 kPa versus 0.15 at the vapor pressure for ethanol). These differences reflect the differential effects of fuel heating and early vaporization in direct-injection and PFI engine designs. Both are appreciably different from the contributions implied by the Honda PMI.

Figure 5-3
Relative Contributions of Hydrocarbons to Sooting Potential



The difference between the dotted lines (E0 gasolines) and the solid lines (E20 gasolines) shows the range of effect that ethanol has on the relative contributions of heavy versus light hydrocarbons. A number of studies (Burke 2018, Chen 2018, Cho 2015) have shown an adverse effect on PM emissions from the ethanol content of a gasoline due to its cooling effect on the fuel charge, which results from ethanol's high heat of vaporization and its tendency to accelerate vaporization of other hydrocarbon compounds in the front half of the distillation curve. The ethanol effect on PM emissions in easily noted in the figure but it is small in comparison to the effect of engine technology.

5.2 Performance of the New PME for SIDI Vehicles

5.2.1 Discussion

Those who have used PME since its publication in CRC Project RW-107-2 will recognize that SIDI coefficients of the New PME are changed only slightly from those of the Old PME in spite of changes in the mathematical formulation. There are two reasons for this:

- The SSI DHAs were used to estimate the prior coefficients for SIDI vehicles. These covered 99.6 to 99.9 wt% of the eight E-94-2 gasolines. Because of this, the calculated PME values were already very close to being 99.9 wt% equivalents. The new expansion factor term has very little effect (only ~1.5% increase in the calculated value).
- The $yTerm_i$ approximation used in the Old PME proved to be a good approximation on average to the YSI values used now, except in the group of heavy, high-sooting compounds where it understated YSI by about 7 percent.

Thus, little has changed since RW-107-2 in the data used to estimate New PME; the resulting empirical coefficients are little changed as well.

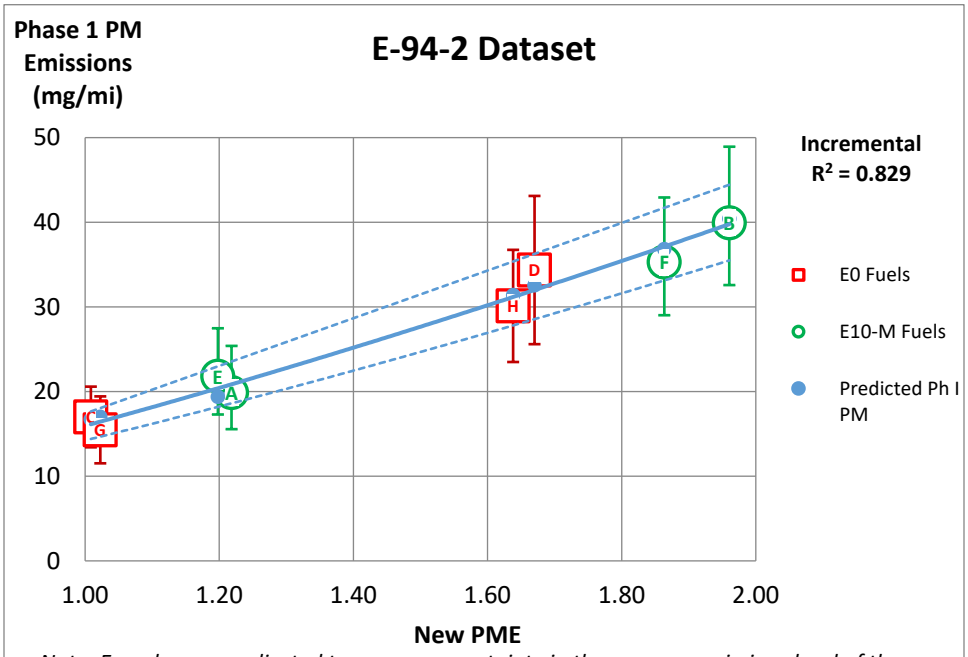
As before, an analysis of the emissions residuals was conducted after the final PME fit to determine whether the bulk properties of the gasolines carried additional explanatory power for PM emissions. RVP and its correlate T05 were found to have a statistically significant relationship to residual emissions, which had also been found in RW-107-2. However, this apparent effect is based on RVP differences of only a few tenths of a psi among the E-94-2 gasolines—a range too narrow to reliably support any conclusion. Further, no RVP effect is found between summer and winter gasolines in the one SIDI vehicle of the SWRI dataset or in New PME's performance for the RVP~9 gasolines in the Growth Energy dataset. No other fuel property indicated any explanatory power for PM emissions whatsoever.

Thus, New PME appears to be a complete index for PM emissions in that it includes all of the information on gasoline that influences emissions. Because it is based on the DHA (which gives the fuel composition) it also includes, in principle at least, all of the information that determines the bulk properties as well. PME is given precedence in explaining emissions, while the test of residuals requires bulk properties to add incremental explanatory that it is not already captured by PME. For example, aromatics content does influence PM emissions, but its effect has already been incorporated in the PME index. RVP and other variables may or may not influence PM emissions, either directly or as surrogate variables, but such effects, if they exist, have already been captured in PME. While alternative PM indices could be developed from correlations of bulk fuel properties to emissions, the work in RW-107 demonstrated that several such correlation-based indices were inferior to PM indices that relied upon itemization of a fuel's hydrocarbon content, whether by DHA or PIONA methods. (CRC RW-107 2019).

5.2.2 Performance of the New PME for the E-94-2 Dataset

Figure 5-4 shows the performance of New PME as a predictor of LA92 Phase I PM emissions in the E-94-2 dataset. The overall trend of PM emissions with New PME is plotted in blue and average emission values by gasoline are plotted in red and green. The error bars in the figure have been adjusted to remove the effect of uncertainty in the overall level of emissions (due to the finite number of measurements). This component of the uncertainty is shared by all values and simply influences where the points and lines are plotted on the vertical axis. By removing this component, the adjusted error bars better indicate the uncertainty in the location of data points relative to the overall trend line.

Figure 5-4
Performance of the New PME in the E-94-2 Emissions Dataset



Note: Error bars are adjusted to remove uncertainty in the average emissions level of the

The direct proportionality of New PME with LA92 Phase I emissions is easily seen overall and for both E0 and E10 gasoline groups. A similar result was found for the Old PME but with a slightly lower incremental R^2 of 0.810. Incremental R^2 measures the ability of the PM index to explain variation in LA92 Phase I PM emissions caused by the gasolines alone without regard to the varying average emission levels of vehicles. The New PME performs better than the Old PME as comparison of the figure with the corresponding Figure 4-3 of the CRC RW-107-2 report will show, albeit by modest amounts.

Table 5-1 compares a series of performance measures for the New PME to measures for the Honda PMI-A[8] from the RW-107 study. Here, the PME index has been fit to the E-94-2 emissions data assuming the existence of direct proportionality with Phase I PM emissions. The PMI index was evaluated in a manner that allowed an empirically fit

[8] PMI-A refers to the Honda PMI evaluated using SSI DHAs.

exponent to improve its match to emissions. The performance differences would be much larger if PME were compared to PMI directly.

The performance measures and error metrics are as follows:

- Incremental R^2 – the conventional R^2 value after removing the contribution to R^2 made by the different average emission levels of the vehicles. The Incremental R^2 measures the ability of the PM index (PME or PMI) to explain variation in LA92 Phase I PM emissions caused by gasolines alone.
- $r_{PEARSON}$ – the usual Pearson correlation coefficient *r* for the concordance of two variables in a dataset.
- $\rho_{SPEARMAN}$ – the Spearman correlation coefficient ρ for the ability of one variable to rank the values of another variable. This is the Pearson *r* applied to the ranks (1 to N) of each variable.
- RMS Error – the root-mean-square error measure for goodness of fit.
- MAE – the maximum absolute error observed.
- Ethanol bias – the percent difference on average between PM emissions for E10 and E0 gasolines.

Table 5-1
New PME Performance Measures for the E-94-2 Emissions Dataset

	New PME This Study		**Honda PMI* RW-107**
Incremental R^2	0.829		0.777
$r_{PEARSON}$	0.99		n/a
$\rho_{SPEARMAN}$	0.95		n/a
Error Metric			
RMS Error	6%		11%
MAE	12%		22%
EtOH Bias	Percent	Prob>|t|	Percent
All Gasolines	2%	0.25	18%
Low PMI	3%	0.045	22%
High PMI	2%	0.37	11%

* After PMI was linearized by an empirically fit exponent.

As the table demonstrates directly, the New PME performs much better than the Honda PMI in all respects, even when PMI is given the benefit of an empirically fit exponent to improve its match to emissions. PME has a substantially higher incremental R^2, RMS and

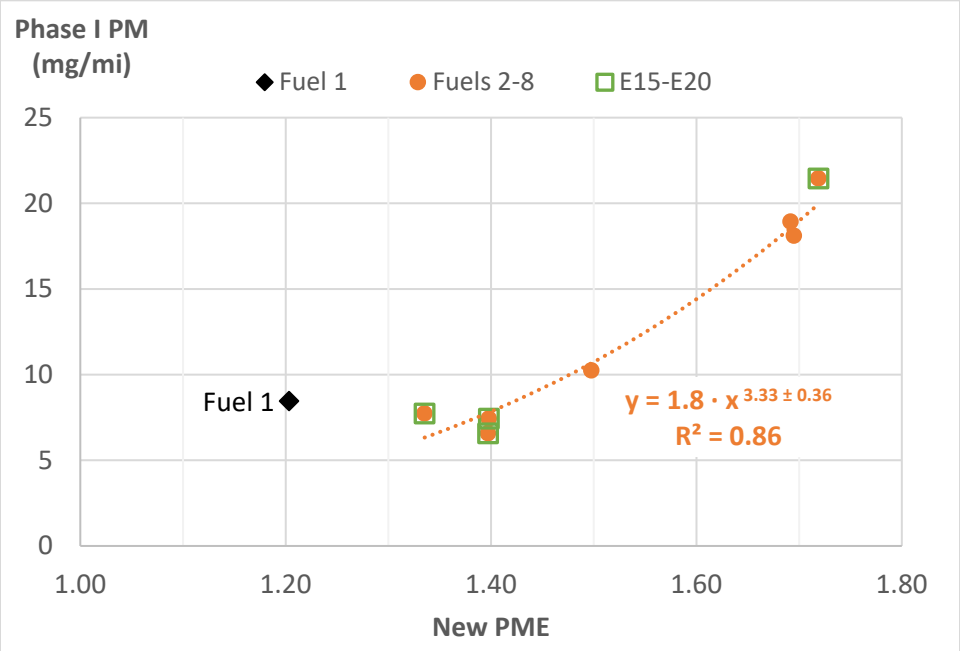
MAE errors approximately nearly one-half that of PMI, and is without ethanol bias. In contrast, PMI has an ethanol bias that ranges from 11 to 22%. The New PME is a large improvement over PMI.

The high $r_{PEARSON}$ and $\rho_{SPEARMAN}$ values of the New PME indicate the predictive power for ranking gasolines. It explains a larger part of the emissions variation among gasolines. Its RMS and MAE errors are reduced from 8% and 16% for the Old PME and it is without an ethanol bias overall and in the Low and High PMI gasolines. The latter is the strongest result. Previously, Fuel E appeared to be significantly different than the other fuels in its response to PME and carried a significant ethanol bias. This has vanished with the improved YSI characterization of sooting potential. The New PME is an evolutionary improvement over the Old PME.

5.2.3 Performance of the New PME in the Growth Energy Dataset

Figure 5-5 plots Phase I PM emissions against the New PME to test whether its revision has resolved the Fuel 1 discrepancy (see Figure 3-5 for a comparable plot using the Old PME). Fuel 1 still stands well to the left of the other fuels at its New PME value of 1.20. Its PME would need to be about 1.40 (17% higher) to place its average emissions data point on the orange trendline. While the Fuel 1 discrepancy motivated the incorporation of YSI into the New PME formulation, doing so does not resolve the Fuel 1 discrepancy.

Figure 5-5
Growth Energy: Phase I PM Emissions versus the New PME



For the other experimental gasolines, New PME performs well for indicating Phase I PM emissions and is generally a modest improvement over the Old PME. The New PME accounts for 86% of the emissions variance versus 0.83 for the Old PME. Finally, the New PME is found to perform well for all four of the E15 and E20 gasolines, boxed in green in

the figure, just as the Old PME did. These include the two match-blended E15 and E20 gasolines in the experiment on aromatics and ethanol content and two splash-blended E15 and E20 gasolines created by adding ethanol to the E10 certification Fuel 3.

In the New PME, the empirical exponent for Growth Energy's Tier 3 vehicles is estimated to be 3.33 ± 0.36, rather than the design value of 1.00. The direct proportionality with Phase I PM emissions has been lost just as for the Old PME. The implication of the larger exponent is that a 10% reduction in the New PME value will translate into a 30% reduction in Phase I PM emissions of these Tier 3 vehicles, rather than the 10% reduction that would occur in Tier 2 vehicles. The larger percentage reduction would be taken off a lower base emissions level in Tier 3 vehicles, but would nevertheless be substantial in mg/mi terms. This remains a conservative outcome in the sense that one can apply PME with confidence to estimate emission reductions from fuel reformulation because the Phase I PM emission reductions for a fleet of Tier 2 and Tier 3 vehicles will be as large or larger than the percentage reduction in the PME value itself.

5.3 Performance of the New PME for PFI Vehicles

5.3.1 Discussion

Unlike the New PME for SIDI vehicles, the coefficients of the New PME for PFI are substantially changed from those of the RW-107-2. A number of factors contribute to this, beginning with the exclusion of 9 of the 27 gasolines from the dataset due to the low wt% of the DHAs available for those fuels. This makes the reduced EPAct dataset used here very different from the complete EPAct dataset that was used before and precludes meaningful comparisons between the prior and current coefficients.

After determination of the New PME coefficients, an analysis of the emissions residuals was conducted to determine whether the bulk properties of the gasolines carried additional explanatory power for PM emissions. Without exception, none of the available bulk properties showed even weak potential to offer explanatory power and this was true whether they were tested individually against the residuals or in a stepwise selection process in which two or more of the variables could jointly demonstrate explanatory power. Included in this were variables—total aromatics content, ethanol, T50, T70, T90, T95 and density—that have been used as predictors for PM.

In these tests, PME is given precedence in explaining emissions, while the test against residuals requires the bulk fuel properties to add incremental explanatory power that it is not already captured by PME. The null finding described above does not mean that variables such as aromatics content, ethanol, T90, and T95 have no effect on emissions, but that their effects have already been captured by the PME index itself. PME appears to be a complete index for PM emissions of PFI vehicles as well.

5.3.2 Performance of the New PME in the Reduced EPAct Dataset

Figure 5-6 shows the performance of New PME as a predictor of LA92 Phase I PM emissions in the reduced EPAct dataset. The overall trend of PM emissions with New PME is plotted in blue and average emission values by fuel are plotted in red and green. The error bars in the figure have been adjusted to remove the effect of uncertainty in the overall level of emissions. This component of the uncertainty is shared by all values and simply influences where the points and lines are plotted on the vertical axis. By removing this component, the adjusted error bars better indicate the uncertainty in the location of data points for fuels relative to the overall trend line.

With one exception (Fuel 11), the data points cluster closely around the power-law trendline with New PME and demonstrate direct proportionality with LA92 Phase I emissions. A similar result was found for PFI vehicles using the Old PME. Here, however, the explanatory power for emissions is substantially increased as indicated by the incremental R^2 of 0.469. This measure was only 0.414 using the Old PME index. Note that it is relatively difficult to achieve high values for the incremental R^2 measure in this dataset because the vehicle emission levels are low and the variability of gravimetric PM emissions measurements is relatively large.

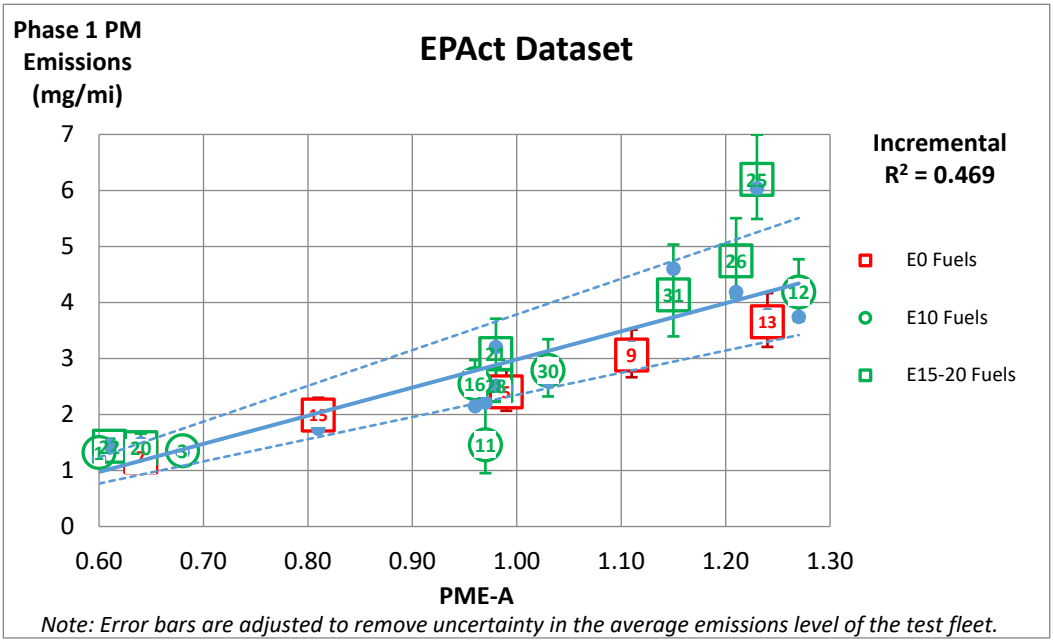
The PM emission residual for Fuel 11 stands off the New PME trendline by a statistically significant amount ($p<<0.01$) just as it did when using the Old PME. With now 18 experimental gasolines, one will exceed the $p=0.01$ threshold by chance alone in one of every 5 or 6 studies. Given this and with just one data point, there is no basis to investigate possible causes with the available data. As for the discrepant Fuel 1 in the Growth Energy study, the Fuel 11 discrepancy remains unresolved.

Table 5-2 compares a series of performance measures for the New PME to measures for the Honda PMI from the RW-107 study. Here, the PME index has been fit to the reduced EPAct emissions data assuming the existence of direct proportionality with emissions. The PMI index was evaluated in a manner that allowed an empirically fit exponent to improve its match to emissions. The performance differences would be much larger if New PME were compared to PMI directly. The performance measures and error metrics are defined in the performance analysis for SIDI vehicles above.

As the table demonstrates directly, the New PME performs much better than the Honda PMI in all respects, even when PMI is given the benefit of an empirically fit exponent. New PME has a substantially higher incremental R^2, RMS and MAE errors approximately nearly one-half that of PMI, and is without ethanol bias. In contrast, PMI has an ethanol bias that ranges from 11 to 22%. The New PME is a large improvement over PMI.

The New PME performs better for indicating Phase I PM emissions in the reduced EPAct dataset than did the Old PME in the complete EPAct dataset (see corresponding Figure 6-3 of the RW-107-2 report). Its high $r_{PEARSON}$ and $\rho_{SPEARMAN}$ values, which indicate its predictive power for ranking gasolines, are nearly on a par with those for SIDI vehicles. The strongest result is that the New PME is without an ethanol bias to a high degree of

Figure 5-6
Performance of the New PME in the Reduced EPAct Dataset



Note: Error bars are adjusted to remove uncertainty in the average emissions level of the test fleet.

Table 5-2
New PME Performance Measures for the Reduced EPAct Dataset

	New PME This Study		Honda PMI* RW-107
Incremental R^2	0.469		0.394
$r_{PEARSON}$	0.94		n/a
$\rho_{SPEARMAN}$	0.97		n/a
Error Metric			
RMS Error	13%		24%
MAE	52%		60%
EtOH Bias	Percent	Prob>|t|	Percent
All Gasolines	1%	0.87	n/a
Low PMI	7%	0.49	n/a
High PMI	-4%	0.52	n/a

* After PMI was linearized by an empirically fit exponent in RW-107.

statistical confidence. Using the Old PME, the measures for ethanol bias were all numerically larger than those found in the table, but without acceptable statistical significance (the strongest being p=0.07). This weaker result (larger effect, but not

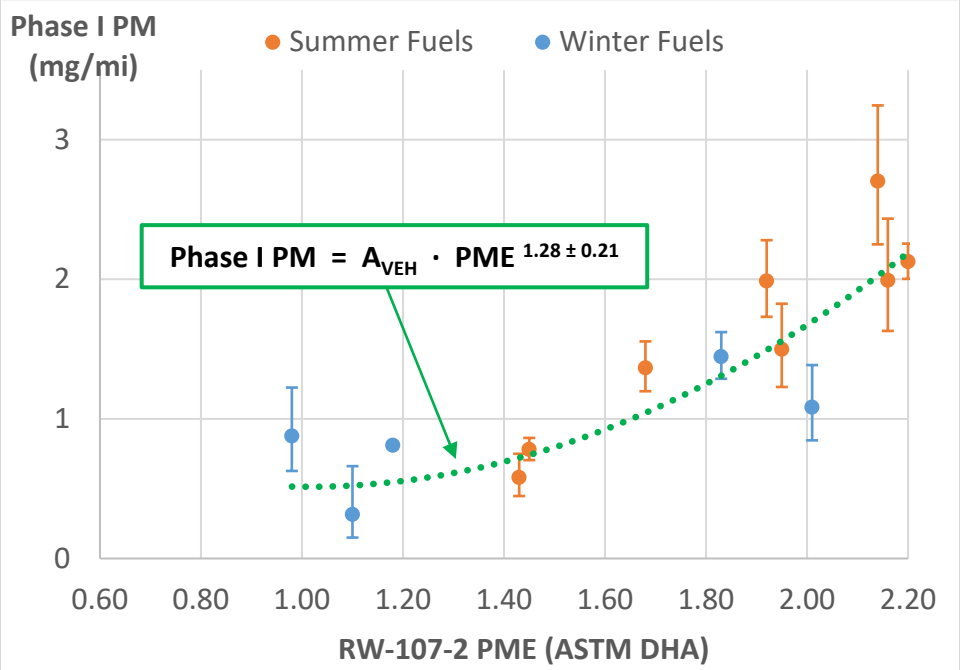
statistically significant) is greatly strengthened with the New PME in which no ethanol bias is present. The New PME for PFI vehicles is a clear-cut improvement over the Old PME.

5.3.3 Performance of the New PME in the SWRI Dataset

The preceding Section 3.3 examined the Old PME's performance in the SWRI dataset. The primary discovery was that the Phase I PM emissions data suggested at least the possibility that PM emissions responded differently to PME in summer versus winter RVP gasolines (previous Figure 3-1). However, the evidence did not meet the p=0.01 threshold for statistical significance used in this work, leading to rejection of the so-called "dual slope" hypothesis (previous Figure 3-2).

Using the New PME, the suggestion of different slopes is further weakened. The two-slope hypothesis now reaches only the p=0.12 level of confidence and cannot be judged statistically significant by any criteria. The single-slope hypothesis shown in Figure 5-7 is confirmed. Although the SWRI dataset consists of only three (Tier 3) PFI vehicles, it

Figure 5-7
SWRI Dataset: Reponse of Winter and Summer Gasoline to New PME



appears that the New PME is applicable across a wide range of RVP values in summer and winter gasolines. The New PME also retains its proportionality with Phase I PM emissions as the slope in the figure is estimated as 1.28 ± 0.21 (1-sigma) and is not statistically different from 1.00 at the 95% confidence level or better.

5.4 Summary

Table 5-3 summarizes the validity and applicability of the New PME based on its performance in the development datasets and the two independent datasets used for validation. It is an effective and unbiased indicator of Phase I PM emissions for both SIDI and PFI vehicles certified to Tier 2 or Tier 3 standards and is demonstrated to be an improved index compared to the Old PME. New PME is an evolutionary improvement for SIDI vehicles and a clear-cut improvement for PFI vehicles.

New PME has been validated for use with E0 through E20 gasolines in both vehicle types and for gasolines with RVP ~ 7 to 9 in SIDI vehicles and 7 ~ 15 in PFI vehicles. For SIDI vehicles, it is likely that it can be used with winter gasolines as well, since no evidence has been found in this or the preceding study that RVP exerts an independent influence on PM emissions that is not accounted for by PME.

Table 5-3
Conclusions on Validity and Applicability of the New PME

	SIDI Vehicles	**PFI Vehicles**
Development dataset	E-94-2 (12 Tier 2 vehicles)	EPAct (15 Tier 2 vehicles)
Validation dataset	Growth Energy 2018 (5 Tier 3 vehicles)	SWRI under RW-107-3 (3 Tier 3 vehicles)
Unbiased indicator of Phase I PM emissions?	Yes [a/]	Yes
Demonstrated Applicability	E0 through E20 RVP ~ 7 to 9 psi	E0 through E20 [b/] RVP ~ 7 through 15 [b/]
Directly Proportional to Phase I PM emissions:		
In Tier 2 vehicles?	Yes, by design	Yes, by design
In Tier 3 vehicles?	No. Exponent of 3.33 ± 0.36	Yes. Exponent of 1.28 ± 0.21

[a/] With the exception of Fuel 1.
[b/] EPAct established PME's range of validity for ethanol as E0 through E20 and for RVP as 7 to 10 psi.

PME is directly proportional to Phase I PM emissions in 3 of the 4 groups so that a 10% reduction in New PME translates to a 10% reduction in emissions. The proportionality is broken for Tier 3 SIDI vehicles in a manner that has a 10% reduction in the index value translates to a 30% reduction in emissions, although taken off a lower base level of emissions for Tier 3 vehicles.

For the Tier 3 SIDI vehicle group, it is reasonable to believe that PME's loss of proportionality and the increased exponent value are the result of changes in engine designs and controls that allowed these vehicles to meet the Tier 3 PM emission standard of 3 mg/mi[9]. Such changes would then translate to reduced PM emissions for all gasolines, including ones with low and intermediate PM potential (whether measured by PMI or PME). However, the percentage reductions would be larger for low and intermediate gasolines and smaller for high PMI/PME gasolines where the inherent propensity of the gasoline to soot is of greater importance. Thus, sharpening of the PM emissions response to PME should be expected.

For Tier 3 PFI vehicles, the empirical exponent differs appreciably from 1.0, but not by a statistically significant amount. This may or may not be an early sign of loss of direct proportionality in more recent PFI vehicles due to changes in engine designs and controls made to reduce PM emissions.

[9] Tier 2 light duty vehicles were subject to a 10-20 mg/mi PM limit as an end-of-life standard and therefore applicable throughout the vehicle lifetime. This is the baseline from which Tier 3 emissions reductions would be made.

6. COMPARISON OF NEW PME TO HONDA PMI

As a final step, this section presents a direct comparison of the New PME to Honda PMI. The term direct means that both indices are treated as "standalone" indicators of vehicle PM emissions without empirical correction or adjustment for their relationships with LA92 Phase I PM emissions. That is how PME was treated in the preceding analysis, which otherwise allowed the Honda PMI to be linearized with respect to PM emissions using empirical correlations. Here, the two indices are assessed on an equal footing.

The viewpoint is that of a fuel designer or blender who must rely on one or the other PM index to control a fuel's propensity to form PM when combusted in a motor vehicle. The PM index, whether the New PME or Honda PMI, is the sole source of information on PM propensity. The following sections explore four different aspects of the relationship between the indices and their relationships to PM emissions.

6.1 The Relationship of the PM Indices

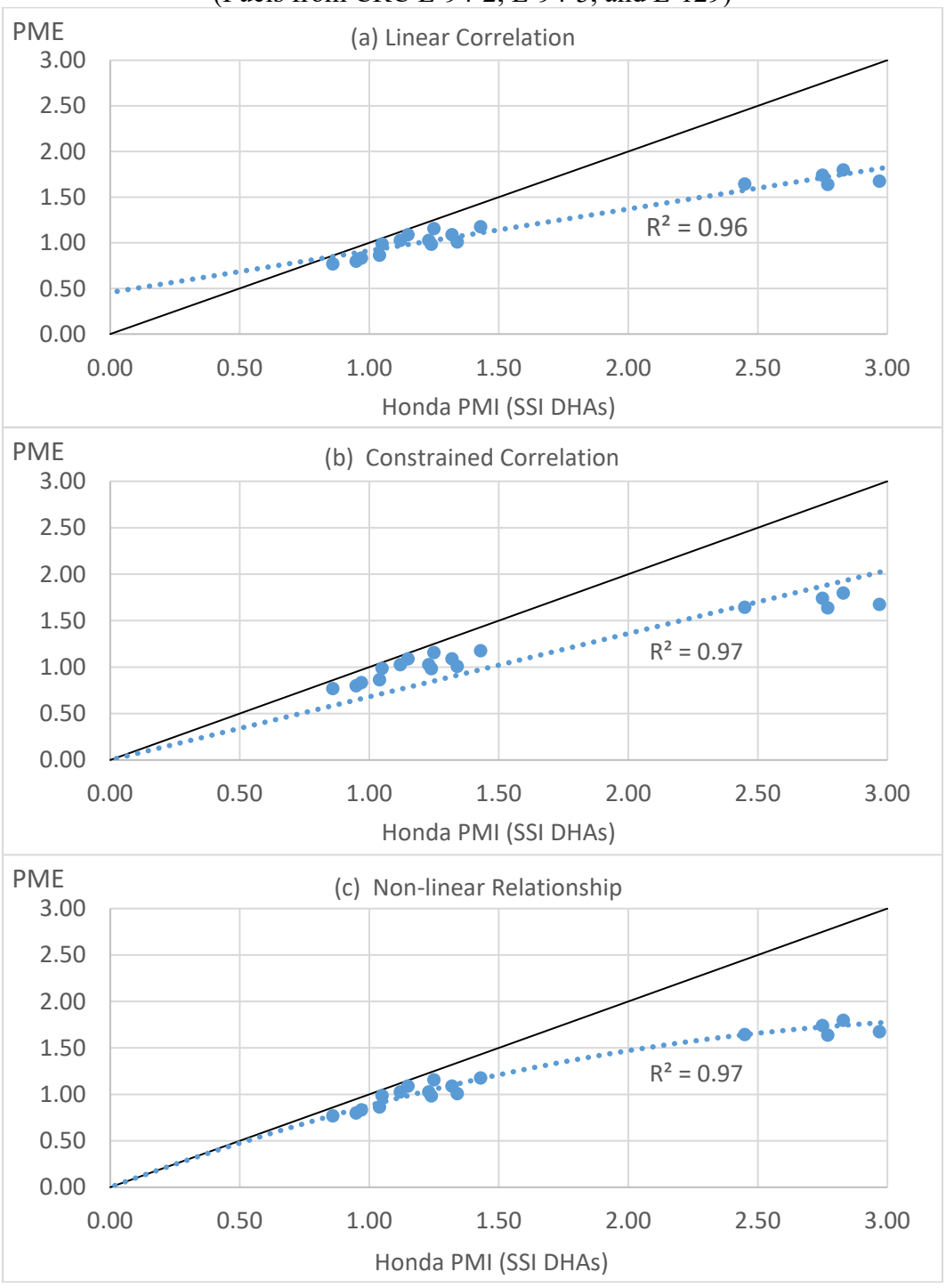
The PM indices have much in common as PME was developed in a process that modified the Honda PMI equation to improve its relationship to PM emissions and its ability to represent a wide variety of gasolines. The result of the process was an enhanced index, the New PME, that was directly proportional to LA92 Phase I PM emissions for not only neat (E0) gasolines but also for gasolines with up to 20 vol% ethanol (E20). It should not be a surprise that the index values from New PME and Honda PMI are highly correlated to each other—to the extent of r~0.98 depending on the dataset. This section explores what that does and does not mean.

Statistical correlations are indicators of the overall relationship between two measures, but they may do little to delineate the nature of the relationship. The three parts of Figure 6-1 are based on the same set of data, which consist of the New PME and Honda PMI values for the experimental fuels in CRC Projects E-94-2, E-94-3 and E-129. SSI DHAs are available for these fuels and cover up to 99.9 wt% of the hydrocarbon compositions. Incomplete characterization of the fuels is not a factor in the comparison of the index values.

The top of Figure 6-1 shows the result of applying conventional linear correlation analysis to the New PME and PMI index values. The index values fall very nearly on a straight line that does an excellent job of capturing their statistical relationship as indicated by the R^2 = 0.96 value. The usual correlation coefficient r is just the square root of R^2 and has the value r=0.979. However, the straight line has a relatively large intercept term that would give a New PME value of 0.50 at a Honda PMI value of 0.00. Such a gasoline would necessarily

Figure 6-1
Relationship of New PME to Honda PMI

(Fuels from CRC E-94-2, E-94-3, and E-129)



be entirely paraffinic (DBE = 0) in order to give a zero or near-zero PMI value[10]. One would not expect such a fuel to have a PME value as large as 0.50 since PME will also trend toward zero as the hydrocarbon composition becomes increasingly paraffinic. Thus, the linear correlation fails to describe the PME/PMI relationship adequately.

A linear correlation line that is constrained to pass through the origin (0, 0) may be a better way of describing the relationship. The usual linear correlation (as in the upper part) passes through the mean value of the dataset, in this case its average values (PME_{AVG}, PMI_{AVG}). Its slope measures how rapidly New PME changes from its average value when PMI moves away from its average. The intercept term of the linear correlation is merely the extrapolation of the slope to the X=0 axis. Referencing the correlation line to the mean value is more distant from the viewpoint of fuel designers and blenders, who wish to control the PM propensity of fuels in an absolute sense. The constrained linear correlation does just that for the two indices – the two indices coincide at the origin and their values imply increased propensity to form PM as one moves away from the origin.

In the middle part of the figure, there remains a strong relationship between the two PM indices (R^2 = 0.97, but see footnote[11]) when the correlation line is constrained to pass through the origin, although some "mis-fit" is now apparent. New PME values lie above the constrained line for PMI values in the range from below 1.00 to 1.50, which is where fuels with low PM propensity would fall. At the far right, where fuels with high PM propensity would fall, the New PME index values tend to lie at and below the constrained line. In fact, New PME values are nearly constant as PMI varies between 2.50 and 3.00. Clearly, New PME and PMI are not equivalent measures in the sense that one can be transformed into the other with high accuracy, even if the high correlation coefficient might suggest otherwise.

The lower part of the figure shows the non-linear relationship between New PME and PMI that has become apparent during the work in this project and its predecessor. The two indices are, in fact, closely related, but that relationship changes as one progresses from low to high index values. Within the range of low PM gasolines near index values of (1.0, 1.0), New PME and PMI have numerically similar values and could be transformed from one to the other with good accuracy. The difference is in how the index values increase as one moves toward high PM gasolines. As one moves from low to mid to high PM gasolines, the Honda PMI value increases more rapidly than does PME, which is what causes the flattening of the curve at its upper end. The rate of increase is also faster than the actual increase in Phase 1 PM emissions, as documented earlier in this report. In contrast, New PME was designed to be proportional to PM emissions.

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[10] An entirely paraffinic gasoline would have a PMI index value of 1/VP, where VP is the geometric mean of the vapor pressures of the paraffinic constituents. The index value would be small, but non-zero. Such a gasoline would have a PME index value that is also small, but non-zero. Both indices approach the origin as the paraffinic nature of a gasoline increases, but the (0,0) values at the origin are not reached.

[11] The R^2 statistic is computed differently than in the unconstrained case, being based on deviations from zero rather than from the dataset mean value. R^2 in the constrained case will generally be a larger value than in the unconstrained case.

While a strong relationship exists between them, the two indices behave differently as one progresses towards high PM gasoline. This tells us that they give different characterizations of the role of heavy hydrocarbons at or near the end of the distillation curve and will give different estimates of the PM emissions reductions that could be achieved by reducing or removing such constituents. At high PMI, a 10% reduction in the Honda PMI index value translates to about a 5% reduction in Phase I PM emissions, while a 10% reduction in New PME translates into a 10% reduction in emissions. Their estimates of the PM propensity of the fuels differ to a sufficient extent that one or the other should be preferred for fuel design and blending. We believe that the inherent proportionality of New PME to Phase I PM emissions makes it the preferred index for such purposes.

6.2 Relationship of the New PME and PMI Indices to Phase I PM Emissions

The performance of the PME index (both the RW-107-3 version and the New PME) was tested in several ways in the preceding sections. One method was to use the PME index as a predictor for LA92 Phase I PM emissions in a regression model that is given in Eq. 6-1 and Eq. 6-2 in two different, but mathematically equivalent forms:

$$\text{Phase I } PM_{i,k} = A_k \cdot PME_i^{\,1.0} \qquad (6\text{-}1)$$

$$\log(\text{Phase I } PM_{i,k}) = \log(A_k) + 1.0 \cdot PME_i \qquad (6\text{-}2)$$

In this, the subscript k denotes vehicle k and the subscript i denotes fuel i.

Conceptually, the models say that Phase I PM emissions in a dataset can be represented as an emission level A_k for each vehicle, at a PME value of 1.0, which is then scaled up/down at other PME levels in proportion to the PME value. PM emissions increase proportionately as a fuel's PME index increases, while PM emissions will trend toward zero as a fuel's PME index decreases and trends toward zero. Such behavior is what one would expect for a PM index that was proportional to emissions.

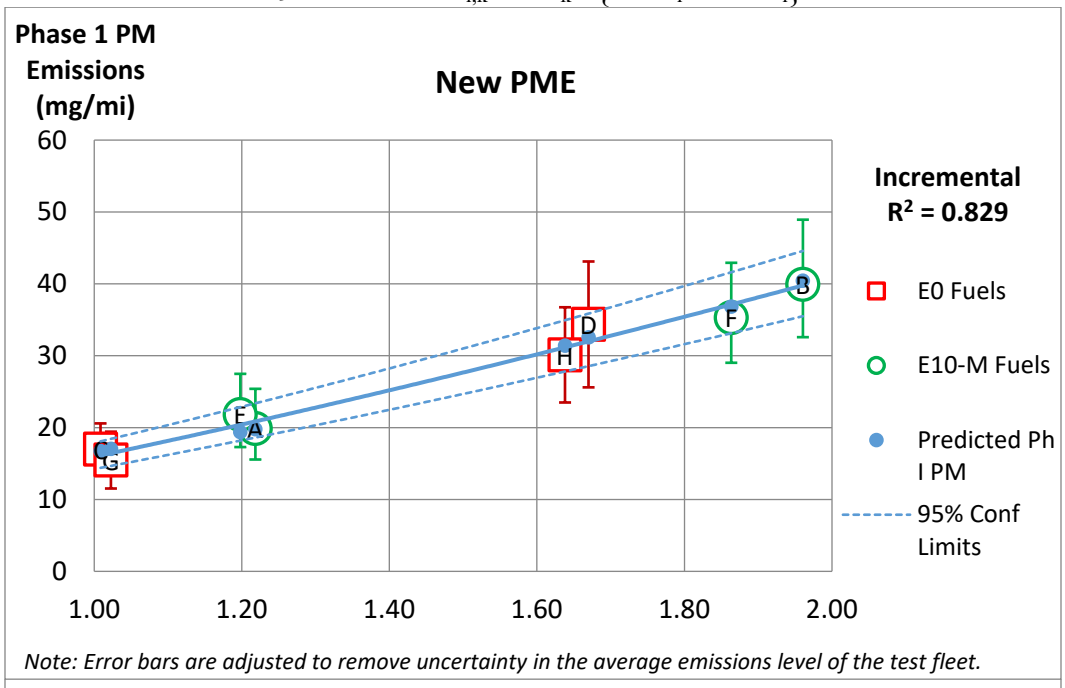
Unlike most regression analysis, the coefficient takes on a fixed value of 1.0 to indicate the direct proportionality of the index to emissions, rather than a variable value that is determined empirically in the regression fit. While unlike most models, these can be fit by a non-linear regression method that allows for constraints on coefficient values. Because the assumption of proportionality is built into the model form, the quality of the fit for an index (whether PME, Honda PMI or another) will be diminished to the extent that the index deviates from true proportionality.

The regression model given in Eqs. 6-1 and 6-2 has been applied to the E-94-2 dataset (SIDI vehicles) and the Reduced EPAct dataset (PFI vehicles) using either the New PME or Honda PMI as the predictive index variable. This is how PME was evaluated in previous sections. But this approach now places PMI on an equal footing, unlike the previous sections where it was allowed an empirical coefficient in place of the fixed 1.0 value to linearize its relationship to Phase I PM emissions.

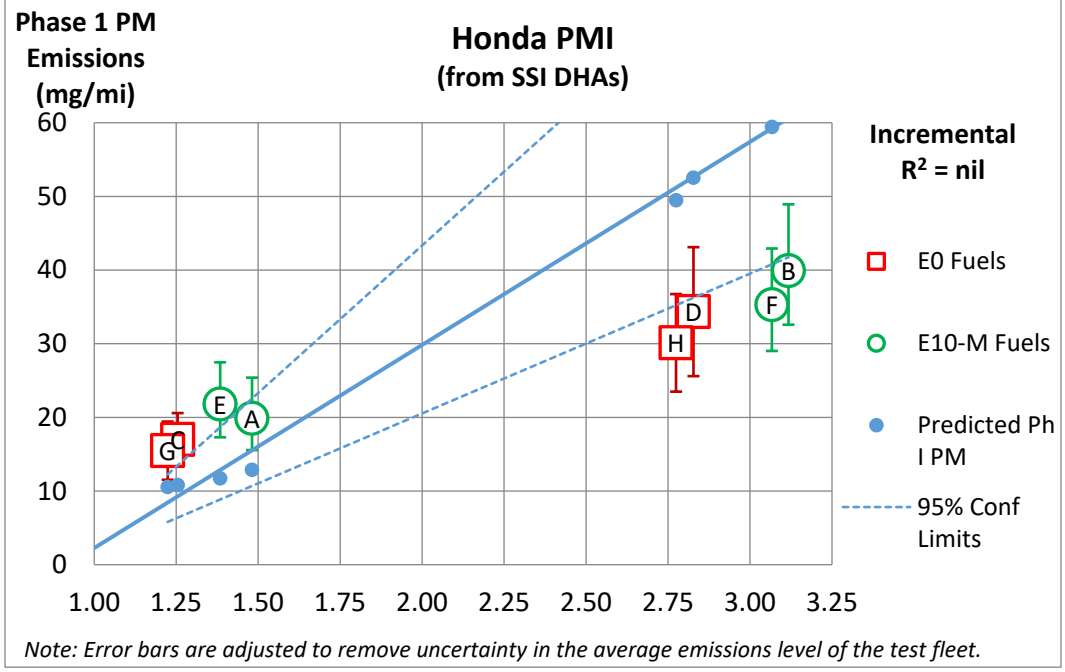
Figure 6-2 shows the performance of both the New PME and the Honda PMI as predictors of LA92 Phase I PM emissions in the E-94-2 dataset. SSI DHAs, with coverages in the range of 99.5 to 99.9 wt%, have been used to evaluate both indices so that differences in coverage rates do not contribute materially to the comparison. The overall trend of PM emissions with New PME is plotted in blue and the average emission values by gasoline

Figure 6-2
Performance of New PME and Honda PMI in the E-94-2 Emissions Dataset

$$\text{LA92 Phase I } PM_{i,k} = A_k \cdot \{PME_i \text{ or } PMI_i\}^{1.0}$$



Note: Error bars are adjusted to remove uncertainty in the average emissions level of the test fleet.



Note: Error bars are adjusted to remove uncertainty in the average emissions level of the test fleet.

are plotted in red and green. The error bars in the figure have been adjusted to remove the effect of uncertainty in the overall level of emissions (due to the finite number of measurements). This format is the same as the preceding Figure 5-4, which can be referenced for comparison.

At the top of the figure, the direct proportionality of New PME with Phase I emissions is easily seen both overall and for the E0 and E10 gasoline groups. The Incremental R^2 = 0.829 value[12] is high by any standard and indicates that New PME does a very good job of indicating a gasoline's potential to form PM when combusted in SIDI vehicles. The data points are clustered around the overall trendline with no apparent difference in fit between the E0 and E10 gasolines. The 95 percent confidence intervals are relatively narrow.

A very different result is seen in the lower portion of the figure for the Honda PMI. When no allowance is made to linearize its relationship with emissions, PMI has essentially no ability to explain variation in Phase I PM emissions beyond the coarse result that gasolines with low index values will have lower PM emissions than gasolines with high index values. The Incremental R^2 is reported as "nil" because the Eq. 6-2 model proves to be a worse fit to the data (higher error sum-of-squares) than one in which only the vehicle intercepts A_k are included. The data points now cluster alternately at the upper- and lower-95 percent confidence limits, which are widely spaced, while the line of predicted Phase PM lies in between. Honda PMI can distinguish Low versus High PM gasolines, but its lack of proportionality with PM emissions limits its ability to indicate finer-grained differences.

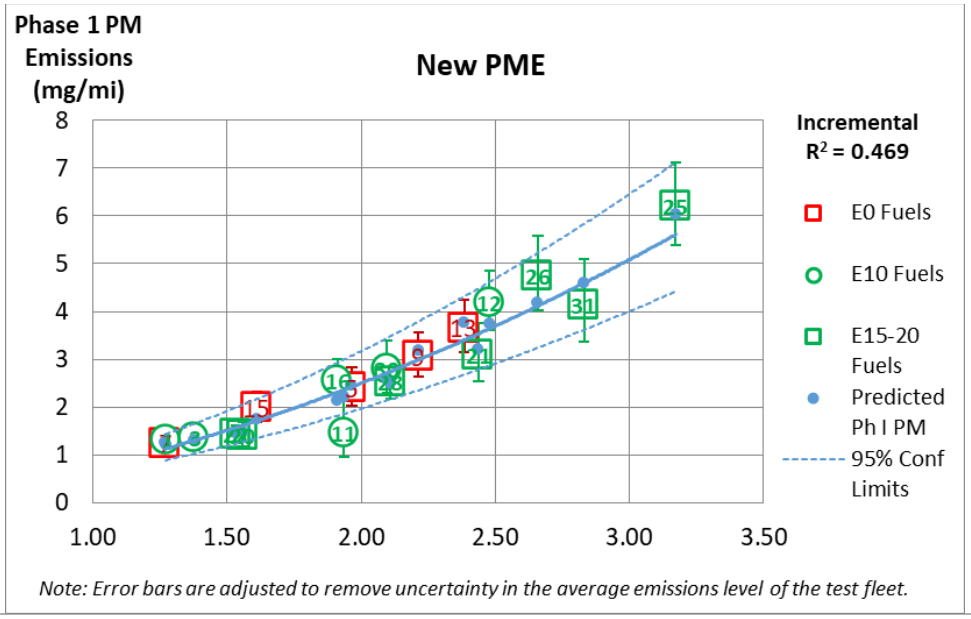
Figure 6-3 presents similar graphs that apply the New PME and Honda PMI to the data of the Reduced EPAct dataset (PFI vehicles). The upper portion shows the performance of the New PME and was previously seen in Figure 5-6. The data points cluster closely around the overall trendline (with one exception), demonstrating the direct proportionality of New PME with LA92 Phase I emissions. Its Incremental R^2 of 0.469 says that it explains not quite one-half of the emissions variability remaining once the contribution of the different emission levels of vehicles is removed. The part that remains unexplained consists largely of errors in PM measurement. Note that it is relatively difficult to achieve high values for the Incremental R^2 because the emission levels of PFI vehicles are low and the variability of gravimetric PM emissions measurement is relatively large.

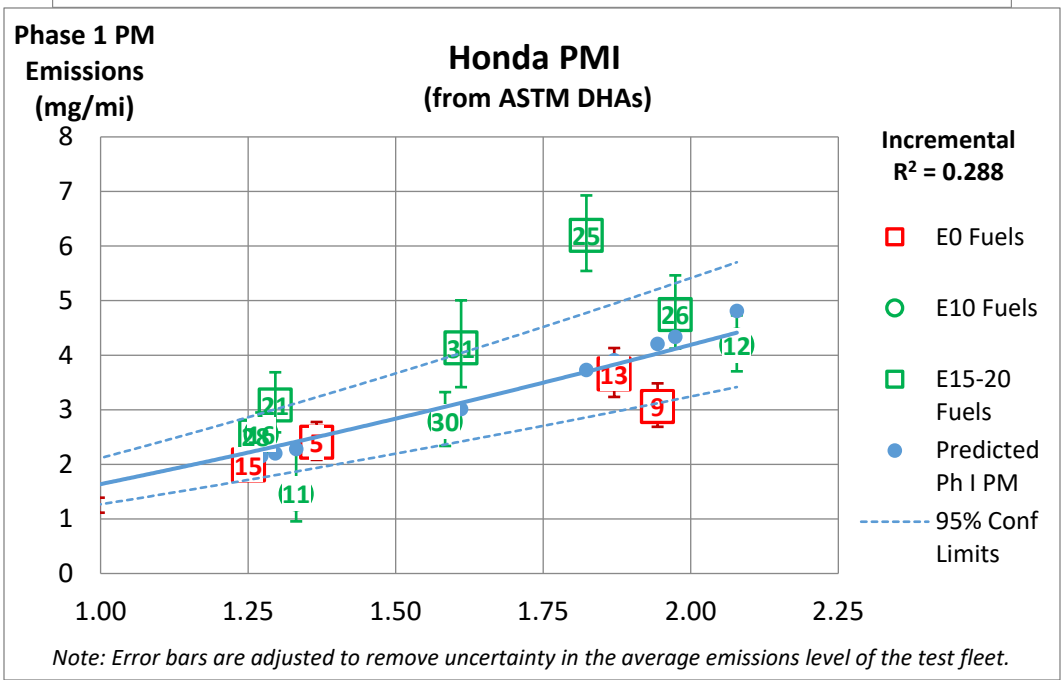
The lower portion of the figure shows the performance of the Honda PMI. In comparison to New PME, there is a substantial scatter of data points around the line of predicted Phase I PM. The Incremental R^2 is only 0.288, substantially lower than for New PME and also reduced from the 0.394 value when it is linearized with respect to emissions (see Table 5-2). PMI performs better in this dataset, for which there are more fuels spanning a nearly-continuous range of index values, than for the SIDI vehicles in the E-94-2 dataset where the fuels largely fell into two groups of low and high index values.

[12] Incremental R^2 measures the ability of the PM index to explain the variation in LA92 Phase I PM emissions caused by the gasolines alone without regard to the varying average emission levels of the vehicles.

Figure 6-3
Performance of New PME and Honda PMI in the Reduced EPACT Emissions Dataset

$$\text{LA92 Phase I } PM_{i,k} = A_k \cdot \{PME_i \text{ or } PMI_i\}^{1.0}$$





Note that the New PME and PMI indices were evaluated using ASTM DHAs, which are the only DHAs in existence for the EPAct fuels. The range of PMI values is reduced compared to those in Figure 6-2, where SSI DHAs were available, because the Honda Equation can be evaluated only to the 98-99 wt% endpoints of the ASTM DHAs, rather than the 99.5-99.9 wt% endpoints typical of SSI DHAs. In contrast, the New PME index

is adjusted to a reference value corresponding to 99.9 wt% and is not materially different when ASTM DHAs are used.

6.3 Measures of New PME Index Performance.

Tables 6-1 and 6-2 compare the performance of the New PME and Honda PMI using a number of performance measures and error metrics as follows:

- Incremental R^2 – a measure of the ability of the PM index (PME or PMI) to explain the variation in LA92 Phase I PM emissions caused by gasoline characteristics alone.
- $r_{PEARSON}$ – the Pearson correlation coefficient *r* for the concordance of two variables in a dataset.
- $\rho_{SPEARMAN}$ – the Spearman correlation coefficient ρ for the ability of one variable to rank the values of another variable.
- RMS Error – the root-mean-square error measure for goodness of fit.
- MAE – the maximum absolute error observed.
- Ethanol bias – the percent difference on average between PM emissions for gasolines of varying ethanol content (E0 and E10 for the E-94-2 dataset and E0, E10, E15 and E20 for the Reduced EPAct dataset).

As Table 6-1 demonstrates for SIDI vehicles (CRC E-94-2 dataset), the New PME performs much better than the Honda PMI in all respects. New PME has a high Incremental R^2 for explaining emissions, while PMI has no such power overall. Both achieve high $r_{PEARSON}$ and $\rho_{SPEARMAN}$ values indicating the predictive power for ranking gasolines, but in the E-94-2 dataset this involves little more than discriminating low versus high PM gasolines.

More to the point, the RMS and MAE errors for PMI are very large – 61% and 86% respectively – compared to the error values for the New PME (6% and 12%, respectively). Both are without apparent ethanol bias, but the result for Honda PMI is largely because, without the benefit of linearization, it does not indicate the PM potential of fuels accurately enough that ethanol-related differences can be seen.

The comparison in Table 6-2 for PFI vehicles (Reduced EPAct dataset) is less stark, but shows clearly the better performance of New PME when PMI is not linearized. New PME is the better index based on measures of the ability to indicate Phase I PM emissions (Incremental R^2) and for ranking gasolines for emissions ($r_{PEARSON}$ and $\rho_{SPEARMAN}$). Both can have large percentage errors (MAE) in the case of an individual fuel, but the RMS error of New PME is only one-half that of PMI. PME has no ethanol bias compared to E0 at any of the ethanol levels (E10, E15, E20)—the average errors are near zero in all cases and there is no evidence of statistical significance. In contrast, PMI has a substantial ethanol bias at the E15 and E20 levels that causes it to underestimate Phase I PM emissions by 31% and 45%, respectively, with good to strong statistical significance in both cases.

Overall, the New PME shows itself to be the preferred PM index in circumstances such as fuel design and/or blending where its proportionality to Phase I PM emissions and applicability to gasolines with a range of ethanol contents would be important. While PMI can perform well when it is linearized empirically to PM emissions, it falls short when linearization is not possible. The Honda PMI has seen widespread use in research since its publication in 2010, but these are also the circumstances where it can be linearized after the fact by fitting an empirical coefficient to the emissions data produced from the work.

6.4 Invariance with Respect to DHA Coverage

A final consideration is that the New PME index is designed to be invariant with respect to detailed differences in the wt% coverage given by different DHAs, while the Honda PMI will yield increasing index values as the wt% coverage of the DHA increases. The effect of varying PMI values will be largest for high PM fuels with increased fractions of heavy hydrocarbons at the end of the distillation curve. In contrast, the index values for New PME have been standardized to a reference coverage of 99.9 wt% and will be little affected

Table 6-1
PM Index Performance Measures for the E-94-2 Emissions Dataset

LA92 Phase I $PM_{i,k} = A_k \cdot \{ PME_i, PMI_i \}^{1.0}$

	New PME		**Honda PMI***	
Incremental R^2	0.829		None	
$r_{PEARSON}$	0.99		0.96	
$\rho_{SPEARMAN}$	0.95		0.98	
Error Metric				
RMS Error	6%		61%	
MAE	12%		86%	
EtOH Bias	Percent	Prob>|t|	Percent	Prob>|t|
All E10	2%	0.25	4%	0.68
Low PMI	3%	0.045	11%	0.04
High PMI	2%	0.37	-2%	0.54
* Without linearization using an empirically fit exponent.				

Table 6-2
PM Index Performance Measures for the Reduced EPAct Dataset

LA92 Phase I $PM_{i,k} = A_k \cdot \{ PME_i, PMI_i \}^{1.0}$

	New PME	**Honda PMI***

Incremental R^2	0.469		0.288	
$r_{PEARSON}$	0.94		0.83	
$\rho_{SPEARMAN}$	0.97		0.88	
Error Metrics				
RMS Error	13%		26%	
MAE	52%		66%	
EtOH Bias	Percent	Prob>|t|	Percent	Prob>|t|
All E10	1%	0.86	2%	0.82
All E15	5%	0.62	31%	0.02
All E20	-3%	0.70	45%	< 0.0001
* Without linearization using an empirically fit exponent.				

by differences in the DHA coverage. The latter is a useful property when one wants to compare old and new work, when the DHA coverage rate has been upgraded over time, and to compare among laboratories where detailed differences in the DHA procedures lead to different coverage rates of the fuels.

Figure 6-4 uses the experimental fuels from CRC Projects E-94-2, E-94-3, and E-129 to illustrate this point. The CRC studies were conducted at SwRI shortly before and after publication of the SSI DHA procedure in CRC AVFL-29 and before the DHA procedure at SwRI had been significantly modified to conform. SSI DHAs were done for the experimental fuels by Separation Systems, Inc. as a compliment to the ASTM DHAs performed by SwRI.

Index values for both the New PMI (in blue) and the Honda PMI (in orange) are plotted in the figure[13]. The index values based on the ASTM DHA procedure form the horizontal axis, while index values based on the SSI DHA procedure form the vertical axis. The ASTM procedure generally achieved 98 to 99 wt% coverage of the hydrocarbons in the fuels, while the SSI procedure achieved 99.5 to as much as 99.9 wt% coverage. The diagonal line (black) is the line of equality between the indices calculated from ASTM and SSI DHAs.

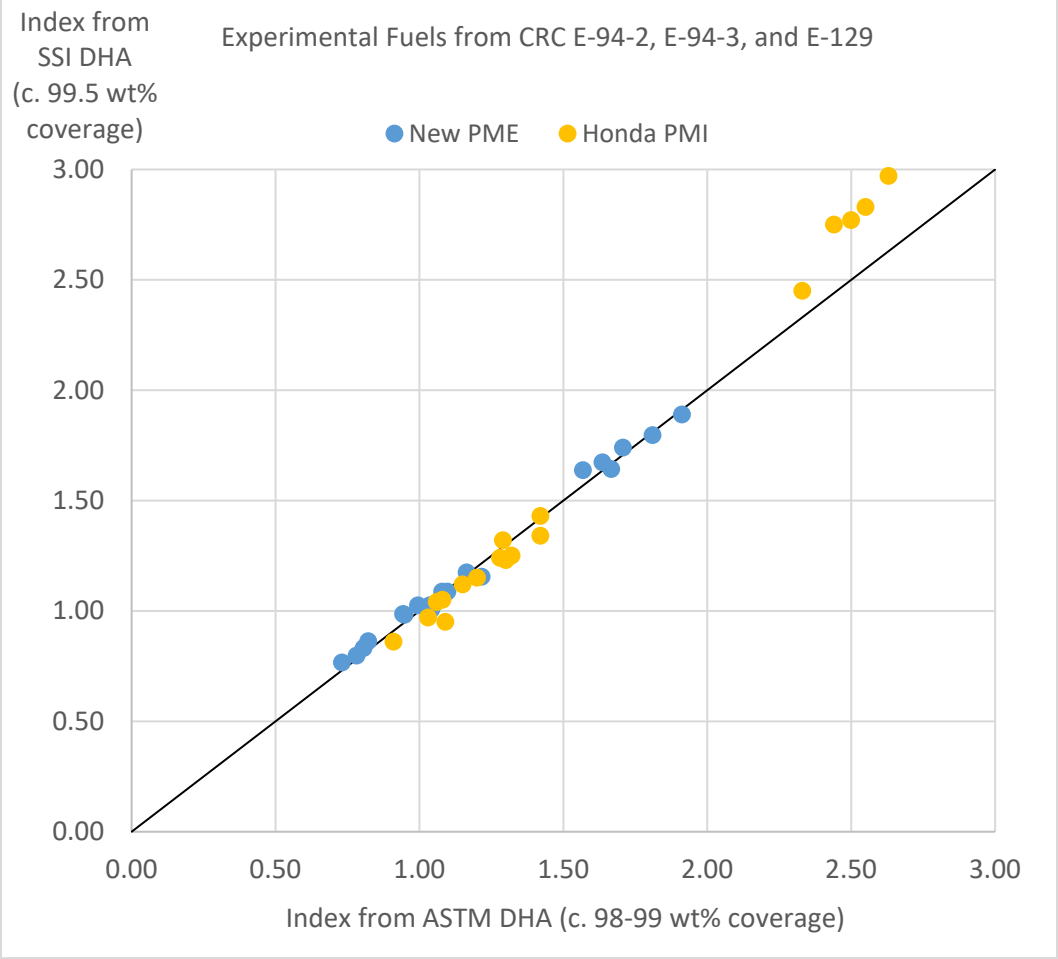
As is apparent, the New PME index values in blue cluster closely along the line of equality. This is because the index value is standardized during its calculation to the value that would be expected at a constant reference coverage of 99.9 wt%. By design, the New PME values are invariant with respect to differences in the wt% coverage of the underlying DHAs in the range from 98 to 99.5 wt%.

[13] The index values are the only applicable to SIDI vehicles, which was the technology tested in the three CRC programs. A similar result would be seen using the index values for PFI vehicles instead.

In contrast, the Honda PMI index values vary from the equality line by amounts that different between low and high index values. In the range from below 1.00 up to 1.50, the PMI index values fall close to the equality line but generally somewhat below. These are fuels with low to moderate propensities to form PM, with relatively fewer heavy hydrocarbons compared to the high PM fuels. The ASTM DHAs provide good characterizations of their hydrocarbon composition that is expanded by the SSI DHA procedure to only a modest extent.

It is a different matter at the upper end of the index range, where the fuels with high PM potential have much larger fractions of heavy hydrocarbons. While the ASTM procedure characterized some of these heavier tails, the SSI procedure was specifically designed to capture much more of them. Because the SSI DHA includes a larger proportion of the heavy hydrocarbons, a numerically larger index value is computed from the Honda PMI equation. High PM gasolines having PMI index values in the range 2.30 to 2.60 when calculated from an ASTM DHA are found to have index values of 2.50 to 3.00 when calculated from an SSI DHA. The Honda PMI is not invariant with respect to the wt% coverage of the underlying DHAs.

Figure 6-4
Influence of DHA wt% Coverage on New PME and Honda PMI Index Values



As has been noted, invariance is a useful property when one wants to compare old and new work, when the DHA coverage rate has been upgraded over time, and to compare among laboratories where detailed differences in the DHA procedures lead to different coverage rates of the fuels. This work (and its predecessor projects) has used DHAs conducted as early as circa 2010 for the EPAct Study, during 2017-18 for the CRC E-94-2, E-94-3 and E-129 projects, and more recently for the new vehicle testing at SwRI under CRC RW-107-3.

More generally, comparison of PM index values across laboratories is complicated not only by differences in wt% coverage rates, but also by the presence of detailed differences in their DHA procedures such as the handling of generic peaks (semi-knowns), the occasional misidentification of known compounds, and any compounds eluting after the end of the method. When the Honda PMI is used as the index, CRC Project AVFL-29-2 showed that such differences could be as large as ± 20% for some fuels (CRC AVFL-29-2, p. 2). Adoption of the New PME in place of PMI should reduce the variability of such comparisons, although other sources of difference will remain.

7. SUMMARY AND DISCUSSION

This report has presented a revised and improved version of the PME index, developed originally in CRC Project RW-107-2 to fill the need for a "new technology" PM index. Table ES-1, reproduced below as Table 7-1, gives its mathematical form and the empirical coefficients needed to compute New PME from DHAs. For SIDI vehicles, the New PME is an evolutionary improvement over the Old PME, but for PFI vehicles it is a clear-cut improvement in the characterization of the PM potential of gasolines. The New PME should be used exclusively as a replacement for the Old PME, which is obsolete.

Figure 7-1
The New PME Formulation

Direct Proportionality

$$\text{LA92 Phase 1 PM} = A_{\text{Veh}} \cdot \text{PME}_{\text{Eng Tech}}^{1.0}$$

Empirical parameters are in orange.

$$\text{PME} = \left(\frac{43.4}{\text{LHV}}\right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot \text{YSI}_i}{VP_i^{\alpha=f(\text{EtOH})}} \right]^{(1+\beta\cdot(99.9-\text{FuelCoverage}_{\text{DHA}}))}$$

$$\alpha = \{ \alpha_{E0}, \alpha_{E10}, \alpha_{E20} \}$$

$$f(\text{EtOH}) = \alpha_{E0} + \Delta\alpha \cdot \text{EtOH}_{\text{VOL\%}}$$

$\text{FuelCoverage}_{\text{DHA}}$ = Total Wt% Identified in DHA

LHV = Lower Heating Value

Engine Technology	DHA Type	N_{TECH}	α_{E0}	α_{E10}	α_{E15}	α_{E20}	β
SIDI	ANY	0.001025	0.451	0.430	0.419[a/]	0.409 [a/]	0.122
PFI	ANY	0.000558	0.257	0.250	0.236	0.222	0.122

[a/] Recommended extension to E15 and E20 based on the α_{E0} to α_{E10} trend.

The index is designed to be directly proportional to Phase I PM emissions in SIDI and PFI vehicles certified to Tier 2 PM emission standards. It retains that proportionality in Tier 3 PFI vehicles, but not in the Tier 3 SIDI vehicles for which significant emission reductions have been made to meet Tier 3 certification standards. New PME provides a conservative estimate of PM emission reductions overall because a percentage reduction made to a gasoline's PME will translate to the same or larger percentage PM emissions reductions from a fleet of Tier 2 and Tier 3 vehicles. It is applicable to a wide range of summer and

winter gasolines in the U.S. market today with ethanol contents ranging from none up to 20 vol%.

The Honda PMI has supported a large body of research on the link between gasolines and PM emissions from motor vehicles over the past decade. The work performed for this project has improved upon the Honda PMI in the following ways:

- The 1+DBE numerator in the Honda PMI has been replaced by YSI values for each compound. YSI was developed at NREL through measurement of soot formation for select hydrocarbon compounds and the modeling of soot formation for the wide range of hydrocarbon compounds found in gasoline.
- The VP term in the denominator has been modified to adopt an exponent α that governs the relative contributions of heavy versus light hydrocarbons to PM emissions in a manner that varies by engine technology (SIDI versus PFI).

In addition, the work has extended the range of fuel effects that it represents. The Honda PMI accounts only for the benefit of ethanol blending—the dilution of gasoline hydrocarbons by an oxygenate that produces little/no soot itself. The New PME formulation addresses this in two ways:

- The α coefficient is made a function of ethanol content to account for the cooling effect caused by ethanol's high heat of vaporization and its effect on the distillation curve. This tends to increase the fractions of heavier hydrocarbons that remain to be combusted in liquid form and, thus, the yield of soot.
- A term has been included to adjust PME for differences in energy content. Gasolines oxygenated with ethanol and many other oxygenated compounds have lower energy contents on a weight basis (per kg) than an E0 or "neat" gasoline. Therefore, a larger quantity of the blended gasoline must be burned to power a vehicle over the drive cycle used to measure PM emissions.

The New PME formulation provides a more complete indication of the PM potential of gasolines and one that can differ substantially from that of the Honda PMI. Appendix C tabulates the New PME values for the experimental gasolines used in this work. Authors of prior research that used the Honda PMI should consider whether conclusions on PM emissions and gasolines could be affected. This is most likely when emissions analysis was done using PMI (or a similar form) as a predictor for PM emissions in work that was intended to identify other factors influencing PM emissions. Examples include Butler 2015 and St. John 2019. The use of New PME instead of PMI should increase the variance explained by the index and leave less to be associated with other variables, which may lead to different conclusions regarding their contributions and statistical significance.

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Appendix A

CRC Project RW-107-3 FINAL REPORT

Note to Reader: the following object will open into the full report when clicked. The pdf version has the SwRI pdf inserted into the RW-107-3a report pdf on a page by page basis.

Final Report

Validation of the New PM Index Formula: Vehicle Testing Phase

Project RW-107-3

Submitted to:

Coordinating Research Council
5755 North Point Parkway, Suite 265
Alpharetta, GA 30022
Attention: Amber Leland

April 2023

POWERTRAIN ENGINEERING DIVISION

Appendix B

MASTER LIST OF HYDROCARBON COMPOUNDS

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
Methane		297	methane	C	CH4	0.0	8.6	outlier	1,683,756.0
Ethane		6324	ethane	CC	C2H6	5.7	8.9	prediction	59,130.7
Methanol	67-56-1	887	methanol	CO	CH4O	6.6	3.0	experiment	1,154.1
Ethene		6325	ethene	C=C	C2H4	8.0	9.8	prediction	103,634.7
Ethanol	64-17-5	702	ethanol	CCO	C2H6O	10.3	2.9	experiment	1,474.6
Propane	74-98-6	6334	propane	CCC	C3H8	12.3	8.9	prediction	14,398.0
1-propanol	71-23-8	1031	propan-1-ol	CCCO	C3H8O	16.2	2.7	experiment	560.9
n-Propanol		1031	propan-1-ol	CCCO	C3H8O	16.2	2.7	experiment	560.9
n-Butane	106-97-8	7843	butane	CCCC	C4H10	18.8	8.8	prediction	5,090.8
i-Propanol		3776	propan-2-ol	CC(C)O	C3H8O	19.2	2.6	experiment	578.9
Propene	115-07-1	8252	prop-1-ene	CC=C	C3H6	21.3	9.0	prediction	16,956.9
1,2-Butadiene		11535	unknown	CC=C=C	C4H6	21.3	9.0	outlier	3,900.9
1-butanol	71-36-3	263	butan-1-ol	CCCCO	C4H10O	22.0	2.5	experiment	352.0
n-Butanol		263	butan-1-ol	CCCCO	C4H10O	22.0	2.5	experiment	352.0
n-Pentane	109-66-0	8003	pentane	CCCCC	C5H12	24.6	2.4	experiment	2,244.6
i-Butane	75-28-5	6360	2-methylpropane	CC(C)C	C4H10	24.7	8.8	prediction	6,655.5
2-butanol	78-92-2	6568	butan-2-ol	CCC(C)O	C4H10O	24.8	2.4	experiment	532.4
2-Butanol		6568	butan-2-ol	CCC(C)O	C4H10O	24.8	2.4	experiment	532.4
1,3 BUTADIENE		7845	buta-1,3-diene	C=CC=C	C4H6	25.7	11.9	prediction	3,919.0
2-methyl-1-propanol	78-83-1	6560	2-methylpropan-1-ol	CC(C)CO	C4H10O	26.2	2.4	experiment	402.8
i-Butanol		6560	2-methylpropan-1-ol	CC(C)CO	C4H10O	26.2	2.4	experiment	402.8
iso-Butanol		6560	2-methylpropan-1-ol	CC(C)CO	C4H10O	26.2	2.4	experiment	402.8
t-Butanol	75-65-0	6386	2-methylpropan-2-ol	CC(C)(C)O	C4H10O	27.5	2.3	experiment	772.1
Butene-1	106-98-9	7844	but-1-ene	CCC=C	C4H8	27.9	9.0	prediction	5,237.4
Cyclobutane		9250	cyclobutane	C1CCC1	C4H8	29.3	8.9	prediction	3,759.4
n-Hexane	110-54-3	8058	hexane	CCCCCC	C6H14	30.4	2.3	experiment	1,062.8
i-Pentane	78-78-4	6556	2-methylbutane	CCC(C)C	C5H12	31.2	8.8	prediction	2,523.3
Methyl-t-butyl ether	1634-04-4	15413	2-methoxy-2-methylpropane	CC(C)(C)OC	C5H12O	31.5	2.2	experiment	1,075.2
Pentene-1	109-67-1	8004	pent-1-ene	CCCC=C	C5H10	34.5	9.0	prediction	2,204.6
c-Butene-2	590-18-1	5287573	(Z)-but-2-ene	CC=CC	C4H8	34.6	9.1	prediction	4,612.1
t-Butene-2	624-64-6	62695	(E)-but-2-ene	CC=CC	C4H8	34.6	9.1	prediction	4,925.5
Isobutene	115-11-7	8255	2-methylprop-1-ene	CC(=C)C	C4H8	36.0	9.2	prediction	5,928.0
3-Methylbutadiene-1,2		11714	unknown	CC(=C=C)C	C5H8	36.0	9.2	outlier	1,872.1
n-Heptane	142-82-5	8900	heptane	CCCCCCC	C7H16	36.0	2.2	experiment	545.8
2,2-Dimethylpropane	463-82-1	17793843	2,2-dimethylpropane	CC(C)(C)C	C5H12	36.3	9.0	prediction	4,250.3
2-Methyl-1,3-Butadiene	78-79-5	6557	2-methylbuta-1,3-diene	CC(=C)C=C	C5H8	36.6	11.2	prediction	2,300.7
2-Methylpentane	107-83-5	7892	2-methylpentane	CCCC(C)C	C6H14	36.7	2.1	experiment	1,301.6
tert-butyl ethyl ether	637-92-3	12512	2-ethoxy-2-methylpropane	CCOC(C)(C)C	C6H14O	37.9	2.1	experiment	777.0
tert-Butyl-Ethyl-Ether		12512	2-ethoxy-2-methylpropane	CCOC(C)(C)C	C6H14O	37.9	2.1	experiment	1,032.4
TAME		0	tert-Amyl methyl ether	CCC(C)(C)OC	C6H14O	38.1	2.1	experiment	717.0
3-Methylpentane	96-14-0	7282	3-methylpentane	CCC(C)CC	C6H14	38.2	2.1	experiment	1,214.8
1,3-Cyclopentadiene	1574-41-0	643785	(3Z)-penta-1,3-diene	CC=CC=C	C5H8	39.0	11.6	prediction	1,838.9
1c,3-Pentadiene		62204	(3E)-penta-1,3-diene	CC=CC=C	C5H8	39.0	11.6	prediction	1,836.8
1t,3-Pentadiene	2004-70-8	62204	(3E)-penta-1,3-diene	CC=CC=C	C5H8	39.0	11.6	prediction	1,838.9
t-1,3-pentadiene	2004-70-8	62204	(3E)-penta-1,3-diene	CC=CC=C	C5H8	39.0	11.6	prediction	1,838.9
Cyclopentane	287-92-3	9253	cyclopentane	C1CCCC1	C5H10	39.4	2.1	experiment	1,637.4
3-Methylbutene-1	563-45-1	11239	3-methylbut-1-ene	CC(C)C=C	C5H10	40.3	9.0	prediction	3,158.3
Cyclopropane, ethyl-	1191-96-4	70933	ethylcyclopropane	CCC1CC1	C5H10	40.9	15.6	prediction	2,199.1
cis 2-pentene	627-20-3	5326160	(Z)-pent-2-ene	CCC=CC	C5H10	41.2	9.1	prediction	2,254.7
c-Pentene-2		5326160	(Z)-pent-2-ene	CCC=CC	C5H10	41.2	9.1	prediction	2,254.7
t-Pentene-2	646-04-8	5326161	(E)-pent-2-ene	CCC=CC	C5H10	41.2	9.1	prediction	2,155.7
1-hexene	592-41-6	11597	hex-1-ene	CCCCC=C	C6H12	42.4	2.0	experiment	1,233.9

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
Hexene-1		11597	hex-1-ene	CCCCC=C	C6H12	42.4	2.0	experiment	1,233.9
2-Methylhexane	591-76-4	11582	2-methylhexane	CCCCC(C)C	C7H16	42.4	2.0	experiment	658.3
2-Methylbutene-1	563-46-2	11240	2-methylbut-1-ene	CCC(=C)C	C5H10	42.5	9.1	prediction	2,455.9
n-Octane	111-65-9	356	octane	CCCCCCCC	C8H18	42.6	2.0	experiment	296.5
Cyclohexane	110-82-7	8078	cyclohexane	C1CCCCC1	C6H12	42.7	2.0	experiment	812.9
2-methyl-1-pentene	763-29-1	12986	2-methylpent-1-ene	CCCC(=C)C	C6H12	42.9	2.0	experiment	1,233.9
2-Methylpentene-1		12986	2-methylpent-1-ene	CCCC(=C)C	C6H12	42.9	2.0	experiment	1,233.9
3-Methylhexane	589-34-4	11507	3-methylhexane	CCCC(C)CC	C7H16	43.0	2.0	experiment	649.5
2,2-Dimethylbutane	75-83-2	6403	2,2-dimethylbutane	CCC(C)(C)C	C6H14	43.4	2.0	experiment	1,670.6
2-methyl-2-butene	513-35-9	10553	2-methylbut-2-ene	CC=C(C)C	C5H10	43.5	2.0	experiment	2,254.7
2-Methylbutene-2		10553	2-methylbut-2-ene	CC=C(C)C	C5H10	43.5	2.0	experiment	2,254.7
1,4-Pentadiene		11587	penta-1,4-diene	C=CCC=C	C5H8	43.5	9.8	prediction	2,575.0
2,3-Dimethylbutane	79-29-8	6589	2,3-dimethylbutane	CC(C)C(C)C	C6H14	44.0	2.0	experiment	1,328.0
Vinyl-Acetylene		12720	but-1-en-3-yne	C=CC#C	C4H4	44.3	11.3	prediction	4,463.5
3-Ethylpentane	617-78-7	12048	3-ethylpentane	CCC(CC)CC	C7H16	44.4	8.8	prediction	626.5
3-methyl-1-pentene	760-20-3	12969	3-methylpent-1-ene	CCC(C)C=C	C6H12	45.1	2.0	experiment	1,404.0
3-Methylpentene-1		12969	3-methylpent-1-ene	CCC(C)C=C	C6H12	45.1	2.0	experiment	1,404.0
1c/t,3-Hexadiene		39175	(3E)-hexa-1,3-diene	CCC=CC=C	C6H10	45.6	11.6	prediction	961.3
Cyclohexene	110-83-8	8079	cyclohexene	C1CCC=CC1	C6H10	45.6	2.0	experiment	728.4
2-ethyl-1-butene	760-21-4	12970	3-methylidenepentane	CCC(=C)CC	C6H12	45.6	2.0	experiment	1,233.9
2-Ethylbutene-1		12970	3-methylidenepentane	CCC(=C)CC	C6H12	45.6	2.0	experiment	1,233.9
2,2-Dimethylpentane	590-35-2	11542	2,2-dimethylpentane	CCCC(C)(C)C	C7H16	47.4	2.0	experiment	865.5
3,3-Dimethylpentane	562-49-2	11229	3,3-dimethylpentane	CCC(C)(C)CC	C7H16	47.7	2.0	experiment	720.3
c-Hexene-2		643835	(Z)-hex-2-ene	CCCC=CC	C6H12	47.8	9.1	prediction	1,087.0
c-Hexene-3	2097470	643783	(Z)-hex-3-ene	CCC=CCC	C6H12	47.8	9.1	prediction	1,087.0
cis 2-hexene	7688-21-3	643835	(Z)-hex-2-ene	CCCC=CC	C6H12	47.8	9.1	prediction	1,087.0
t-Hexene-2		639661	(E)-hex-2-ene	CCCC=CC	C6H12	47.8	9.1	prediction	1,081.9
t-Hexene-3		638066	(E)-hex-3-ene	CCC=CCC	C6H12	47.8	9.1	prediction	1,138.8
trans 2-hexene		639661	(E)-hex-2-ene	CCCC=CC	C6H12	47.8	9.1	prediction	1,081.9
trans 3-hexene	13269-52-8	638066	(E)-hex-3-ene	CCC=CCC	C6H12	47.8	9.1	prediction	1,138.8
4-Methylheptane	589-53-7	11512	4-methylheptane	CCCC(C)CCC	C8H18	48.1	2.0	experiment	356.9
1-heptene	592-76-7	11610	hept-1-ene	CCCCCC=C	C7H14	48.4	2.0	experiment	608.4
Heptene-1		11610	hept-1-ene	CCCCCC=C	C7H14	48.4	2.0	experiment	608.4
3-Methylheptane	589-81-1	11519	3-methylheptane	CCCCC(C)CC	C8H18	48.7	2.0	experiment	341.6
2-methyl-1-hexene	6094-02-6	22468	2-methylhex-1-ene	CCCCC(=C)C	C7H14	49.1	2.0	experiment	646.6
2-Methylhexene-1	1531866	22468	2-methylhex-1-ene	CCCCC(=C)C	C7H14	49.1	2.0	experiment	646.6
2,3-Dimethylpentane	565-59-3	11260	2,3-dimethylpentane	CCC(C)C(C)C	C7H16	49.4	2.0	experiment	662.8
2-Methylheptane	592-27-8	11594	2-methylheptane	CCCCCC(C)C	C8H18	49.4	2.0	experiment	351.2
2,4-Dimethylpentane	108-08-7	7907	2,4-dimethylpentane	CC(C)CC(C)C	C7H16	49.6	2.0	experiment	816.6
1,3-Pentadiene, 2-methyl-, (E)-		638070	(3E)-2-methylpenta-1,3-diene	CC=CC(=C)C	C6H10	50.0	10.9	prediction	923.4
C6-Diolefin-1	1528-30-9	638070	(3E)-2-methylpenta-1,3-diene	CC=CC(=C)C	C6H10	50.0	10.9	prediction	913.2
n-Nonane	111-84-2	8141	nonane	CCCCCCCCC	C9H20	50.1	2.0	experiment	157.5
1,5-Hexadiene		11598	hexa-1,5-diene	C=CCCC=C	C6H10	50.1	9.7	prediction	1,348.8
4-methyl-1-pentene	691-37-2	12724	4-methylpent-1-ene	CC(C)CC=C	C6H12	50.2	2.0	experiment	1,338.3
4-Methylpentene-1		12724	4-methylpent-1-ene	CC(C)CC=C	C6H12	50.2	2.0	experiment	1,484.1
4-Methylpentene-1-trans		12724	4-methylpent-1-ene	CC(C)CC=C	C6H12	50.2	2.0	experiment	1,338.3
Methylcyclopentane	96-37-7	7296	methylcyclopentane	CC1CCCC1	C6H12	50.3	2.0	experiment	991.8
3-Ethylhexane	619-99-8	12096	3-ethylhexane	CCCC(CC)CC	C8H18	51.0	8.8	prediction	352.8
2,2-Dimethylhexane	590-73-8	11551	2,2-dimethylhexane	CCCCC(C)(C)C	C8H18	52.8	2.0	experiment	462.4
3,3-dimethyl-1-butene	558-37-2	11210	3,3-dimethylbut-1-ene	CC(C)(C)C=C	C6H12	53.1	2.0	experiment	1,962.1
3,3-Dimethylbutene-1		11210	3,3-dimethylbut-1-ene	CC(C)(C)C=C	C6H12	53.1	2.0	experiment	1,962.1
2,3-dimethyl-1-butene	563-78-0	11249	2,3-dimethylbut-1-ene	CC(C)C(=C)C	C6H12	53.4	2.0	experiment	1,422.9
2,3-Dimethylbutene-1		11249	2,3-dimethylbut-1-ene	CC(C)C(=C)C	C6H12	53.4	2.0	experiment	1,422.9

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
3-Ethylpentene-1		19951	3-ethylpent-1-ene	CCC(CC)C=C	C7H14	53.4	9.0	prediction	731.7
3-Methylhexene-1	3404-61-3	18848	3-methylhex-1-ene	CCCC(C)C=C	C7H14	53.4	9.0	prediction	731.7
5-Methylhexene-1	3524-73-0	77058	5-methylhex-1-ene	CC(C)CCC=C	C7H14	53.4	9.0	prediction	733.3
2-methyl-2-pentene	625-27-4	12243	2-methylpent-2-ene	CCC=C(C)C	C6H12	53.6	2.0	experiment	1,096.5
2-Methylpentene-2		12243	2-methylpent-2-ene	CCC=C(C)C	C6H12	53.6	2.0	experiment	1,096.5
Methylcyclohexane	108-87-2	7962	methylcyclohexane	CC1CCCCC1	C7H14	53.6	2.0	experiment	515.8
2-Pentene-c&t-, 4-methyl-		12659	4-methylpent-2-ene	CC=CC(C)C	C6H12	53.6	9.2	prediction	1,310.3
2-Pentene-CIS- ,4-methyl		5326159	(Z)-4-methylpent-2-ene	CC=CC(C)C	C6H12	53.6	9.2	prediction	1,379.2
4-Methyl-t-pentene-2	674-76-0	172092	(E)-4-methylpent-2-ene	CC=CC(C)C	C6H12	53.6	9.2	prediction	1,097.7
4-Methyl-t-pentene-2-E		172092	(E)-4-methylpent-2-ene	CC=CC(C)C	C6H12	53.6	9.2	prediction	1,097.7
cis 4-methyl-2-pentene	691-38-3	5326159	(Z)-4-methylpent-2-ene	CC=CC(C)C	C6H12	53.6	9.2	prediction	1,379.2
4-Methyl-1,3-pentadiene	926-56-7	13555	4-methylpenta-1,3-diene	CC(=CC=C)C	C6H10	53.6	11.5	prediction	893.0
C10_I-Paraffins(18)		15600	decane	CCCCCCCCCC	C10H22	54.0	2.7	experiment	106.2
C10_I-Paraffins(19)		15600	decane	CCCCCCCCCC	C10H22	54.0	2.7	experiment	106.2
C10_I-Paraffins(20)		15600	decane	CCCCCCCCCC	C10H22	54.0	2.7	experiment	129.6
n-Decane	124-18-5	15600	decane	CCCCCCCCCC	C10H22	54.0	2.7	experiment	88.9
Cyclopropane, butyl-	930-57-4	70257	butylcyclopropane	CCCCC1CC1	C7H14	54.1	15.6	prediction	537.3
2-Heptene	592-77-8	11611	hept-2-ene	CCCCC=CC	C7H14	54.4	9.1	prediction	544.6
c-Heptene-2		643836	(Z)-hept-2-ene	CCCCC=CC	C7H14	54.4	9.1	prediction	545.8
c-Heptene-3	2097503	5357258	(Z)-hept-3-ene	CCCC=CCC	C7H14	54.4	9.1	prediction	597.5
t-Heptene-2	14686-13-6	639662	(E)-hept-2-ene	CCCCC=CC	C7H14	54.4	9.1	prediction	651.4
t-Heptene-3		5357259	(E)-hept-3-ene	CCCC=CCC	C7H14	54.4	9.1	prediction	580.2
trans 3-heptene	14686-14-7	5357259	(E)-hept-3-ene	CCCC=CCC	C7H14	54.4	9.1	prediction	580.2
3,4-Dimethylhexane	583-48-2	11412	3,4-dimethylhexane	CCC(C)C(C)CC	C8H18	55.2	2.0	experiment	360.2
2,2,3-Trimethylbutane	464-06-2	10044	2,2,3-trimethylbutane	CC(C)C(C)(C)C	C7H16	55.3	2.0	experiment	794.9
2-Ethylpentene-1		520668	3-methylidenehexane	CCCC(=C)CC	C7H14	55.7	9.1	prediction	633.7
4-methyl-1-hexene	3769-23-1	19589	4-methylhex-1-ene	CCC(C)CC=C	C7H14	55.8	2.0	experiment	731.7
4-Methylhexene-1		19589	4-methylhex-1-ene	CCC(C)CC=C	C7H14	55.8	2.0	experiment	731.7
2-Pentene, 3-methyl-		12014	3-methylpent-2-ene	CCC(=CC)C	C6H12	55.8	9.1	prediction	1,164.4
3-methyl-2-pentene	922-61-2	12014	3-methylpent-2-ene	CCC(=CC)C	C6H12	55.8	9.1	prediction	1,164.4
3-Methyl-c-pentene-2	922-62-3	643935	(Z)-3-methylpent-2-ene	CCC(=CC)C	C6H12	55.8	9.1	prediction	1,086.7
3-Methyl-t-pentene-2		642661	(E)-3-methylpent-2-ene	CCC(=CC)C	C6H12	55.8	9.1	prediction	1,164.4
3,3-Dimethylhexane	563-16-6	11233	3,3-dimethylhexane	CCCC(C)(C)CC	C8H18	56.0	9.0	prediction	408.7
3-Methyl-3-ethylpentane	1067-08-9	14018	3-ethyl-3-methylpentane	CCC(C)(CC)CC	C8H18	56.0	9.0	prediction	348.8
1-octene	111-66-0	8125	oct-1-ene	CCCCCCC=C	C8H16	56.0	2.0	experiment	323.9
Octene-1		8125	oct-1-ene	CCCCCCC=C	C8H16	56.0	2.0	experiment	323.9
2,4-Dimethylhexane	589-43-5	11511	2,4-dimethylhexane	CCC(C)CC(C)C	C8H18	56.1	2.0	experiment	425.0
2,5-Dimethylhexane	592-13-2	11592	2,5-dimethylhexane	CC(C)CCC(C)C	C8H18	56.1	2.0	experiment	427.9
1-Heptene, 2-methyl-		27519	2-methylhept-1-ene	CCCCCC(=C)C	C8H16	56.6	2.0	experiment	351.2
1,6-Heptadiene		16968	hepta-1,6-diene	C=CCCCC=C	C7H12	56.7	9.7	prediction	632.2
2,3-Dimethylhexane	584-94-1	11447	2,3-dimethylhexane	CCCC(C)C(C)C	C8H18	56.8	8.9	prediction	373.7
2-Methyl-3-ethylpentane	609-26-7	11863	3-ethyl-2-methylpentane	CCC(CC)C(C)C	C8H18	56.8	8.9	prediction	373.7
1c/t,4-Hexadiene		5365552	(4E)-hexa-1,4-diene	CC=CCC=C	C6H10	56.8	9.6	prediction	1,154.1
2-Methyloctane	3221-61-2	18591	2-methyloctane	CCCCCCC(C)C	C9H20	57.5	8.8	prediction	192.7
3-Methyloctane	2216-33-3	16664	3-methyloctane	CCCCCC(C)CC	C9H20	57.5	8.8	prediction	191.7
4-Ethylheptane	2216-32-2	16663	4-ethylheptane	CCCC(CC)CCC	C9H20	57.5	8.8	prediction	202.6
4-Methyloctane	2216-34-4	16665	4-methyloctane	CCCCC(C)CCC	C9H20	57.5	8.8	prediction	200.6
Heptane, 3-ethyl-	15869-80-4	51806	3-ethylheptane	CCCCC(CC)CC	C9H20	57.5	8.8	prediction	194.1
2-Methyl-1,4-pentadiene		12987	2-methylpenta-1,4-diene	CC(=C)CC=C	C6H10	58.2	9.7	prediction	1,410.3
3,3-Dimethylpentene-1	3404-73-7	18852	3,3-dimethylpent-1-ene	CCC(C)(C)C=C	C7H14	58.5	9.2	prediction	833.2
Butyne-2		10419	but-2-yne	CC#CC	C4H6	58.6	11.3	prediction	2,787.2
Ethylcyclopentane	1640-89-7	15431	ethylcyclopentane	CCC1CCCC1	C7H14	58.6	2.0	experiment	486.2
1,3-Octadiene		517653	(3E)-octa-1,3-diene	CCCCC=CC=C	C8H14	58.7	11.6	prediction	279.1

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
3,4-Dimethylpentene-1	7385-78-6	23866	3,4-dimethylpent-1-ene	CC(C)C(C)C=C	C7H14	59.3	9.2	prediction	833.2
3-ethyl-2-pentene	816-79-5	13159	3-ethylpent-2-ene	CCC(=CC)CC	C7H14	59.8	2.0	experiment	611.1
3-Ethylpentene-2		13159	3-ethylpent-2-ene	CCC(=CC)CC	C7H14	59.8	2.0	experiment	611.1
1-Heptene, 3-methyl-		20946	3-methylhept-1-ene	CCCCC(C)C=C	C8H16	60.0	9.0	prediction	396.7
1-Heptene, 5-methyl-	13151-04-7	99888	5-methylhept-1-ene	CCC(C)CCC=C	C8H16	60.0	9.0	prediction	396.7
C11_I-Paraffins(23)		14257	undecane	CCCCCCCCCCC	C11H24	60.1	3.0	experiment	65.5
n-Undecane	1120-21-4	14257	undecane	CCCCCCCCCCC	C11H24	60.1	3.0	experiment	51.8
(Z)-4-Methyl-2-hexene	3683-19-0	5357251	(Z)-4-methylhex-2-ene	CCC(C)C=CC	C7H14	60.2	9.1	prediction	684.0
2-Hexene, 4-methyl-, (E)-	3683-22-5	5357249	(E)-4-methylhex-2-ene	CCC(C)C=CC	C7H14	60.2	9.1	prediction	684.0
2-Methyl-c-hexene-3	15840-60-5	5365948	(Z)-2-methylhex-3-ene	CCC=CC(C)C	C7H14	60.2	9.1	prediction	684.0
2-Methyl-t-hexene-3		5352548	(E)-2-methylhex-3-ene	CCC=CC(C)C	C7H14	60.2	9.1	prediction	722.7
2-Methyl-t-hexene-3(1)		5352548	(E)-2-methylhex-3-ene	CCC=CC(C)C	C7H14	60.2	9.1	prediction	684.0
4-Methyl-t/c-hexene-2	3404-55-5	5357249	(E)-4-methylhex-2-ene	CCC(C)C=CC	C7H14	60.2	9.1	prediction	684.0
5-Methyl-c-hexene-2	13151-17-2	5364850	(Z)-5-methylhex-2-ene	CC=CCC(C)C	C7H14	60.2	9.1	prediction	684.0
5-Methyl-t-hexene-2	7385-82-2	5357252	(E)-5-methylhex-2-ene	CC=CCC(C)C	C7H14	60.2	9.1	prediction	657.9
cis-2-Methyl-hexene-3		5365948	(Z)-2-methylhex-3-ene	CCC=CC(C)C	C7H14	60.2	9.1	prediction	684.0
2,3-Dimethylheptane	3074-71-3	26375	2,3-dimethylheptane	CCCCC(C)C(C)C	C9H20	60.2	2.0	experiment	206.0
Ethylcyclohexane	1678-91-7	15504	ethylcyclohexane	CCC1CCCCC1	C8H16	60.7	2.0	experiment	267.6
2,3,4-Trimethylpentane	565-75-3	11269	2,3,4-trimethylpentane	CC(C)C(C)C(C)C	C8H18	60.9	2.0	experiment	386.8
1,3-Pentadiene, 2,3-dimethyl-		137118	2,3-dimethylpenta-1,3-diene	CC=C(C)C(=C)C	C7H12	60.9	13.5	prediction	705.7
3-Octene, (Z)-	14850-22-7	5362722	(Z)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	326.1
C8 - Iso-Olefin - 3		638228	(E)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	178.0
C8_Iso-Olefins(1)		5356796	(Z)-oct-2-ene	CCCCCC=CC	C8H16	60.9	9.1	prediction	352.8
C8_Iso-Olefins(3)		638228	(E)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	178.0
C8_Iso-Olefins(4)		5356796	(Z)-oct-2-ene	CCCCCC=CC	C8H16	60.9	9.1	prediction	333.0
c-Octene-2	2097322	5356796	(Z)-oct-2-ene	CCCCCC=CC	C8H16	60.9	9.1	prediction	293.8
c-Octene-3		5362722	(Z)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	311.0
c-Octene-4		5364446	(Z)-oct-4-ene	CCCC=CCCC	C8H16	60.9	9.1	prediction	326.1
t-4-Octene		5357253	(E)-oct-4-ene	CCCC=CCCC	C8H16	60.9	9.1	prediction	317.1
t-Octene-2	111-23-6	5364448	(E)-oct-2-ene	CCCCCC=CC	C8H16	60.9	9.1	prediction	326.1
t-Octene-3		638228	(E)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	326.1
t-Octene-4		5357253	(E)-oct-4-ene	CCCC=CCCC	C8H16	60.9	9.1	prediction	315.7
trans 2-octene	13389-42-9	5364448	(E)-oct-2-ene	CCCCCC=CC	C8H16	60.9	9.1	prediction	326.1
trans 3-octene	14919-01-8	638228	(E)-oct-3-ene	CCCCC=CCC	C8H16	60.9	9.1	prediction	326.1
trans 4-octene	14850-23-8	5357253	(E)-oct-4-ene	CCCC=CCCC	C8H16	60.9	9.1	prediction	315.7
Cyclohexene, 4-methyl-		11572	4-methylcyclohexene	CC1CCC=CC1	C7H12	61.0	3.0	experiment	477.4
Isopropylcyclobutane		136673	propan-2-ylcyclobutane	CC(C)C1CCC1	C7H14	61.5	8.9	prediction	569.8
1-Pentene, 2,3-dimethyl-	3404-72-6	18851	2,3-dimethylpent-1-ene	CCC(C)C(=C)C	C7H14	61.5	9.2	prediction	736.6
2,4-Dimethylpentene-1	2213-32-3	16657	2,4-dimethylpent-1-ene	CC(C)CC(=C)C	C7H14	61.5	9.2	prediction	736.6
2-Ethyl-3-methylbutene-1		81818	2-methyl-3-methylidenepentane	CCC(=C)C(C)C	C7H14	61.5	9.2	prediction	736.6
2,2,4-Trimethylpentane	540-84-1	10907	2,2,4-trimethylpentane	CC(C)CC(C)(C)C	C8H18	61.7	2.0	experiment	550.8
2,2,3-Trimethylpentane	564-02-3	11255	2,2,3-trimethylpentane	CCC(C)C(C)(C)C	C8H18	61.8	9.0	prediction	420.1
2,3,3-Trimethylpentane	560-21-4	11215	2,3,3-trimethylpentane	CCC(C)(C)C(C)C	C8H18	61.8	9.0	prediction	375.5
1-methyl-1-cyclohexene	591-49-1	11574	1-methylcyclohexene	CC1=CCCCC1	C7H12	62.0	3.0	experiment	419.2
C7_Naphtheno-Olefins(1)		11574	1-methylcyclohexene	CC1=CCCCC1	C7H12	62.0	3.0	experiment	419.2
C7_Naphtheno-Olefins(3)		11574	1-methylcyclohexene	CC1=CCCCC1	C7H12	62.0	3.0	experiment	419.2
C7-Naphtho-olefin-1		11574	1-methylcyclohexene	CC1=CCCCC1	C7H12	62.0	3.0	experiment	419.2
Cyclohexene, 1-methyl-		11574	1-methylcyclohexene	CC1=CCCCC1	C7H12	62.0	3.0	experiment	419.2
2-Ethylhexene-1		15404	3-methylideneheptane	CCCCC(=C)CC	C8H16	62.3	9.2	prediction	351.2
C8_Iso-Olefins(2)		15404	3-methylideneheptane	CCCCC(=C)CC	C8H16	62.3	9.2	prediction	352.8
Heptane, 4-methylene-		519193	4-methylideneheptane	CCCC(=C)CCC	C8H16	62.3	9.2	prediction	460.8
2-Methyl-2-hexene	2738-19-4	17656	2-methylhex-2-ene	CCCC=C(C)C	C7H14	62.4	9.1	prediction	584.2
3-Methyl-3-hexene		5352447	(E)-3-methylhex-3-ene	CCC=C(C)CC	C7H14	62.4	9.1	prediction	560.6

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
3-Methyl-c-hexene-2	10574-36-4	5357248	(Z)-3-methylhex-2-ene	CCCC(=CC)C	C7H14	62.4	9.1	prediction	559.6
3-Methyl-c-hexene-3	4914-89-0	5357250	(Z)-3-methylhex-3-ene	CCC=C(C)CC	C7H14	62.4	9.1	prediction	611.1
3-Methyl-t-hexene-2	20710-38-8	5352660	(E)-3-methylhex-2-ene	CCCC(=CC)C	C7H14	62.4	9.1	prediction	653.2
3-Methyl-t-hexene-3	3899-36-3	5352447	(E)-3-methylhex-3-ene	CCC=C(C)CC	C7H14	62.4	9.1	prediction	609.8
2,2-Dimethylheptane		14062	2,2-dimethylheptane	CCCCCC(C)(C)C	C9H20	62.6	9.0	prediction	252.6
3,3-Diethylpentane	1067-20-5	14020	3,3-diethylpentane	CCC(CC)(CC)CC	C9H20	62.6	9.0	prediction	175.1
3,3-Dimethylheptane		520991	3,3-dimethylheptane	CCCCC(C)(C)CC	C9H20	62.6	9.0	prediction	224.6
C9_I-Paraffins(2)		14062	2,2-dimethylheptane	CCCCCC(C)(C)C	C9H20	62.6	9.0	prediction	255.3
Heptane, 2,2-dimethyl-		14062	2,2-dimethylheptane	CCCCCC(C)(C)C	C9H20	62.6	9.0	prediction	252.6
Heptane, 3,3-dimethyl-		520991	3,3-dimethylheptane	CCCCC(C)(C)CC	C9H20	62.6	9.0	prediction	223.2
n-Propylcyclopentane		16270	propylcyclopentane	CCCC1CCCC1	C8H16	63.0	8.9	prediction	257.7
1c,2-Dimethylcyclopentane	1192-18-3	14498	(1S,2R)-1,2-dimethylcyclopentane	CC1CCCC1C	C7H14	63.0	9.3	prediction	560.9
1c,3-Dimethylcyclopentane	2532-58-3	17326	(1S,3R)-1,3-dimethylcyclopentane	CC1CCC(C1)C	C7H14	63.0	9.3	prediction	648.0
1t,2-Dimethylcyclopentane	822-50-4	252359	(1R,2R)-1,2-dimethylcyclopentane	CC1CCCC1C	C7H14	63.0	9.3	prediction	632.2
1t,3-Dimethylcyclopentane	1759-58-6	15656	(1R,3R)-1,3-dimethylcyclopentane	CC1CCC(C1)C	C7H14	63.0	9.3	prediction	635.0
2,4-Dimethylheptane	1071-26-7	16656	2,4-dimethylheptane	CCCC(C)CC(C)C	C9H20	63.4	8.9	prediction	242.5
2,5-Dimethylheptane	2216-30-0	16662	2,5-dimethylheptane	CCC(C)CCC(C)C	C9H20	63.4	8.9	prediction	230.2
2,6-Dimethylheptane	1072-05-5	14069	2,6-dimethylheptane	CC(C)CCCC(C)C	C9H20	63.4	8.9	prediction	233.5
3,4-Dimethylheptane	922-28-1	13534	3,4-dimethylheptane	CCCC(C)C(C)CC	C9H20	63.4	8.9	prediction	205.5
3,5-Dimethylheptane	926-82-9	13558	3,5-dimethylheptane	CCC(C)CC(C)CC	C9H20	63.4	8.9	prediction	229.1
C9_I-Paraffins(3)		16656	2,4-dimethylheptane	CCCC(C)CC(C)C	C9H20	63.4	8.9	prediction	247.6
C9_I-Paraffins(4)		13558	3,5-dimethylheptane	CCC(C)CC(C)CC	C9H20	63.4	8.9	prediction	229.1
Hexane, 3-ethyl-2-methyl-	16789-46-1	86067	3-ethyl-2-methylhexane	CCCC(CC)C(C)C	C9H20	63.4	8.9	prediction	216.5
1,4-Heptadiene		5367564	(4E)-hepta-1,4-diene	CCC=CCC=C	C7H12	63.4	9.6	prediction	615.6
1,5-Heptadiene	1541-23-7	5364394	(5E)-hepta-1,5-diene	CC=CCCC=C	C7H12	63.4	9.6	prediction	652.4
2-Methylnonane		13379	2-methylnonane	CCCCCCCC(C)C	C10H22	64.1	8.8	prediction	111.0
3-Ethyloctane	5881-17-4	79985	3-ethyloctane	CCCCCC(CC)CC	C10H22	64.1	8.8	prediction	109.6
3-Methylnonane	1465084	22202	3-methylnonane	CCCCCCC(C)CC	C10H22	64.1	8.8	prediction	106.2
4-Methylnonane	17301-94-8	28455	4-methylnonane	CCCCCC(C)CCC	C10H22	64.1	8.8	prediction	111.0
5-Methylnonane	15869-85-9	27518	5-methylnonane	CCCCC(C)CCCC	C10H22	64.1	8.8	prediction	113.5
C10_I-Paraffins(16)		22202	3-methylnonane	CCCCCCC(C)CC	C10H22	64.1	8.8	prediction	106.2
C10_I-Paraffins(17)		22202	3-methylnonane	CCCCCCC(C)CC	C10H22	64.1	8.8	prediction	106.2
1-nonene	124-11-8	31285	non-1-ene	CCCCCCCC=C	C9H18	64.4	2.0	experiment	176.3
Nonene-1		31285	non-1-ene	CCCCCCCC=C	C9H18	64.4	2.0	experiment	176.3
2-Pentene, 4,4-dimethyl-		5326158	(E)-4,4-dimethylpent-2-ene	CC=CC(C)(C)C	C7H14	65.2	9.3	prediction	889.0
4,4-Dimethyl-c-pentene-2		5326157	(Z)-4,4-dimethylpent-2-ene	CC=CC(C)(C)C	C7H14	65.2	9.3	prediction	700.5
4,4-Dimethyl-t-pentene-2		5326158	(E)-4,4-dimethylpent-2-ene	CC=CC(C)(C)C	C7H14	65.2	9.3	prediction	889.0
C7 - Iso-Olefin - 2		5326158	(E)-4,4-dimethylpent-2-ene	CC=CC(C)(C)C	C7H14	65.2	9.3	prediction	630.0
C7_Iso-Olefins(2)		5326158	(E)-4,4-dimethylpent-2-ene	CC=CC(C)(C)C	C7H14	65.2	9.3	prediction	630.0
2,4-Octadiene		5367588	(2E,4E)-octa-2,4-diene	CCCC=CC=CC	C8H14	65.5	12.0	prediction	258.9
1-Octene, 3-methyl-		518715	3-methyloct-1-ene	CCCCCC(C)C=C	C9H18	66.6	9.0	prediction	220.6
1-Octene, 4-methyl-		518717	4-methyloct-1-ene	CCCCC(C)CC=C	C9H18	66.6	9.0	prediction	220.6
1-Octene, 6-methyl-	13151-10-5	518716	6-methyloct-1-ene	CCC(C)CCCC=C	C9H18	66.6	9.0	prediction	220.6
C9_Iso-Olefins(5)		518716	6-methyloct-1-ene	CCC(C)CCCC=C	C9H18	66.6	9.0	prediction	220.6
3-Heptene, 2-methyl-		5357255	(E)-2-methylhept-3-ene	CCCC=CC(C)C	C8H16	66.8	9.1	prediction	372.0
4-Ethyl-2-hexene		5352665	(E)-4-ethylhex-2-ene	CCC(CC)C=CC	C8H16	66.8	9.1	prediction	369.5
4-Methyl-2-heptene	3404-56-6	5352648	(E)-4-methylhept-2-ene	CCCC(C)C=CC	C8H16	66.8	9.1	prediction	372.0
4-methyl-2-heptene(1)		5352648	(E)-4-methylhept-2-ene	CCCC(C)C=CC	C8H16	66.8	9.1	prediction	372.0
5-Methyl-3-heptene		5462826	(E)-5-methylhept-3-ene	CCC=CC(C)CC	C8H16	66.8	9.1	prediction	391.2
Butane, 2,2,3,3-tetramethyl-	594-82-1	11675	2,2,3,3-tetramethylbutane	CC(C)(C)C(C)(C)C	C8H18	66.8	9.7	prediction	451.0
n-Dodecane	112-40-3	8182	dodecane	CCCCCCCCCCCC	C12H26	67.1	3.4	experiment	31.1
4-Nonene	2198-23-4	94226	non-4-ene	CCCCC=CCCC	C9H18	67.5	9.1	prediction	181.9
C9_Iso-Olefins(4)		5364590	(E)-non-2-ene	CCCCCCC=CC	C9H18	67.5	9.1	prediction	176.3

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
cis-3-Nonene	20237-46-1	5364453	(Z)-non-3-ene	CCCCCC=CCC	C9H18	67.5	9.1	prediction	227.3
cis-4-Nonene	10405-84-2	5364456	(Z)-non-4-ene	CCCCC=CCCC	C9H18	67.5	9.1	prediction	181.9
c-Nonene-2		5364455	(Z)-non-2-ene	CCCCCCC=CC	C9H18	67.5	9.1	prediction	162.1
c-Nonene-3	20237-46-0	5364453	(Z)-non-3-ene	CCCCCC=CCC	C9H18	67.5	9.1	prediction	227.3
t-Nonene-2	6434-78-2	5364590	(E)-non-2-ene	CCCCCCC=CC	C9H18	67.5	9.1	prediction	189.5
t-Nonene-3	20063-92-7	5364445	(E)-non-3-ene	CCCCCC=CCC	C9H18	67.5	9.1	prediction	181.9
trans-4-Nonene	10405-85-3	5364454	(E)-non-4-ene	CCCCC=CCCC	C9H18	67.5	9.1	prediction	227.3
1,4-Pentadiene, 3,3-dimethyl-	1112-35-2	136863	3,3-dimethylpenta-1,4-diene	CC(C)(C=C)C=C	C7H12	67.5	9.9	prediction	861.6
1,3-dimethyl-c-cyclohexane	638-04-0	252361	(1R,3S)-1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	332.2
1,3-dimethylcyclohexane	591-21-9	11564	1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	290.4
1,3-Dimethylcyclohexane,c&t		11564	1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	290.4
1,3-dimethyl-t-cyclohexane		11564	1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	308.6
1,4-dimethylcyclohexane	589-90-2	11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	324.6
1c,3-Dimethylcyclohexane		11564	1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	334.2
1c,4-Dimethylcyclohexane	624-29-3	11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	290.4
1t,3-Dimethylcyclohexane	2207-03-6	16629	(1R,3R)-1,3-dimethylcyclohexane	CC1CCCC(C1)C	C8H16	67.6	2.1	experiment	290.4
1t,4-Dimethylcyclohexane		11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	337.3
1t,4t-Dimethylcyclohexane		11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	337.7
C8_Mono-Naphthenes(2)		11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	290.4
Cyclohexane c&t, 1,4-dimethyl-		11523	1,4-dimethylcyclohexane	CC1CCC(CC1)C	C8H16	67.6	2.1	experiment	324.6
1,1-Dimethylcyclohexane	590-66-9	11549	1,1-dimethylcyclohexane	CC1(CCCCC1)C	C8H16	67.9	2.1	experiment	348.8
C8_Mono-Naphthenes(1)		11549	1,1-dimethylcyclohexane	CC1(CCCCC1)C	C8H16	67.9	2.1	experiment	337.7
C8_Mono-Naphthenes(5)		11549	1,1-dimethylcyclohexane	CC1(CCCCC1)C	C8H16	67.9	2.1	experiment	273.7
2,3-Dimethyl-1-hexene	16746-86-4	86061	2,3-dimethylhex-1-ene	CCCC(C)C(=C)C	C8H16	68.1	9.2	prediction	399.5
2-Pentene, 3-ethyl-2-methyl-		140591	3-ethyl-2-methylpent-1-ene	CCC(CC)C(=C)C	C8H16	68.1	9.2	prediction	399.5
Hexane, 2-methyl-4-methylene-		520670	2-methyl-4-methylidenehexane	CCC(=C)CC(C)C	C8H16	68.1	9.2	prediction	465.5
2-Pentene, 2,4-dimethyl-	625-65-0	12260	2,4-dimethylpent-2-ene	CC(C)C=C(C)C	C7H14	68.2	9.1	prediction	765.2
2-Pentene, 3,4-dimethyl-, (E)-	4914-92-5	638068	(E)-3,4-dimethylpent-2-ene	CC=C(C)C(C)C	C7H14	68.2	9.1	prediction	659.7
2-Pentene, 3,4-dimethyl-, (Z)-	4914-91-4	643784	(Z)-3,4-dimethylpent-2-ene	CC=C(C)C(C)C	C7H14	68.2	9.1	prediction	659.7
3,4-Dimethyl-c-pentene-2		643784	(Z)-3,4-dimethylpent-2-ene	CC=C(C)C(C)C	C7H14	68.2	9.1	prediction	699.5
C7 - Iso-Olefin - 1		12260	2,4-dimethylpent-2-ene	CC(C)C=C(C)C	C7H14	68.2	9.1	prediction	765.2
C7_Iso-Olefins(1)		12260	2,4-dimethylpent-2-ene	CC(C)C=C(C)C	C7H14	68.2	9.1	prediction	765.2
1,1-Dimethylcyclopentane	1638-26-2	15421	1,1-dimethylcyclopentane	CC1(CCCC1)C	C7H14	68.3	11.4	prediction	698.0
C7 - MonoNaph - 1		15421	1,1-dimethylcyclopentane	CC1(CCCC1)C	C7H14	68.3	11.4	prediction	616.1
C7_Mono-Naphthenes(1)		15421	1,1-dimethylcyclopentane	CC1(CCCC1)C	C7H14	68.3	11.4	prediction	698.0
2,2,3-Trimethylhexane	16747-25-4	28021	2,2,3-trimethylhexane	CCCC(C)C(C)(C)C	C9H20	68.4	9.0	prediction	241.9
2,2,4-Trimethylhexane	16747-26-5	28022	2,2,4-trimethylhexane	CCC(C)CC(C)(C)C	C9H20	68.4	9.0	prediction	293.1
2,2,5-Trimethylhexane	3522-94-9	19041	2,2,5-trimethylhexane	CC(C)CCC(C)(C)C	C9H20	68.4	9.0	prediction	302.8
C9 - MonoNapth - 5		28022	2,2,4-trimethylhexane	CCC(C)CC(C)(C)C	C9H20	68.4	9.0	prediction	196.8
C9_I-Paraffins(1)		19041	2,2,5-trimethylhexane	CC(C)CCC(C)(C)C	C9H20	68.4	9.0	prediction	245.9
C9_I-Paraffins(5)		19041	2,2,5-trimethylhexane	CC(C)CCC(C)(C)C	C9H20	68.4	9.0	prediction	261.7
C9_I-Paraffins(6)		19041	2,2,5-trimethylhexane	CC(C)CCC(C)(C)C	C9H20	68.4	9.0	prediction	276.5
C9-Isoparaffin-x		19041	2,2,5-trimethylhexane	CC(C)CCC(C)(C)C	C9H20	68.4	9.0	prediction	284.6
Hexane, 2,3,3-trimethyl-	16747-28-7	28023	2,3,3-trimethylhexane	CCCC(C)(C)C(C)C	C9H20	68.4	9.0	prediction	219.1
Hexane, 2,4,4-trimethyl-	16747-30-1	28024	2,4,4-trimethylhexane	CCC(C)(C)CC(C)C	C9H20	68.4	9.0	prediction	276.5
Hexane, 3,3,4-trimethyl-		28025	3,3,4-trimethylhexane	CCC(C)C(C)(C)CC	C9H20	68.4	9.0	prediction	210.4
1-Pentene, 2,4,4-trimethyl-	25167-70-8	7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	508.8
2,4,4-trimethyl-1-pentene	107-39-1	7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	504.8
C8 - IsoOlefin - 10		7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	266.1
C8 - IsoOlefin - 4		7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	363.7
C8 - IsoOlefin - 5		7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	342.2
C8 - IsoOlefin - 7		7868	2,4,4-trimethylpent-1-ene	CC(=C)CC(C)(C)C	C8H16	68.5	2.1	experiment	313.1
i-Propylcyclopentane	3875-51-2	19751	propan-2-ylcyclopentane	CC(C)C1CCCC1	C8H16	68.8	9.0	prediction	295.1

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3-Methylcyclopentene	1120-62-3	14263	3-methylcyclopentene	CC1CCC=C1	C6H10	68.8	9.6	prediction	1,156.7
4-methylcyclopentene	1759-81-5	15658	4-methylcyclopentene	CC1CC=CC1	C6H10	68.8	9.6	prediction	1,136.3
2-Methyloctene-1	4588-18-5	78335	2-methyloct-1-ene	CCCCCCC(=C)C	C9H18	68.8	9.2	prediction	195.9
C9_Iso-Olefins(2)		78335	2-methyloct-1-ene	CCCCCCC(=C)C	C9H18	68.8	9.2	prediction	195.9
2-Heptene, 3-methyl-		5366149	(E)-3-methylhept-2-ene	CCCCC(=CC)C	C8H16	69.0	9.1	prediction	333.0
3-Ethyl-3-Hexene	16789-51-8	140138	3-ethylhex-3-ene	CCC=C(CC)CC	C8H16	69.0	9.1	prediction	365.2
3-Heptene, 3-methyl-		5364638	(E)-4-methylhept-3-ene	CCCC(=CCC)C	C8H16	69.0	9.1	prediction	333.0
3-Heptene, 4-methyl-	4485-16-9	5364638	(E)-4-methylhept-3-ene	CCCC(=CCC)C	C8H16	69.0	9.1	prediction	333.0
2,2-Dimethyloctane	15869-87-1	85150	2,2-dimethyloctane	CCCCCCC(C)(C)C	C10H22	69.1	9.0	prediction	141.5
3-Ethyl-3-methylheptane	17302-01-1	140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	116.0
C10 - IsoParaffin - 1		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	186.6
C10 - IsoParaffin - 2		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	188.6
C10 - IsoParaffin - 5		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	107.4
C10 - IsoParaffin - 6		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	106.1
C10 Isoparaffin -1		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	136.2
C10_I-Paraffins(1)		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	127.4
C10_I-Paraffins(22)		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	141.0
C10_I-Paraffins(23)		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	167.3
C10_I-Paraffins(24)		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	177.7
C10_I-Paraffins(25)		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	177.7
C10_I-Paraffins(5)		85150	2,2-dimethyloctane	CCCCCCC(C)(C)C	C10H22	69.1	9.0	prediction	177.7
C10_I-Paraffins(6)		85150	2,2-dimethyloctane	CCCCCCC(C)(C)C	C10H22	69.1	9.0	prediction	177.7
C10-isoparaffin-x		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	UNKN
C10-isoparaffin-x		140213	3-ethyl-3-methylheptane	CCCCC(C)(CC)CC	C10H22	69.1	9.0	prediction	186.6
Octane, 3,3-dimethyl-	4110-44-5	138117	3,3-dimethyloctane	CCCCCC(C)(C)CC	C10H22	69.1	9.0	prediction	125.6
2,3,4-Trimethylhexane	921-47-1	13533	2,3,4-trimethylhexane	CCC(C)C(C)C(C)C	C9H20	69.2	9.2	prediction	216.0
2,3,5-Trimethylhexane	1069-53-0	14045	2,3,5-trimethylhexane	CC(C)CC(C)C(C)C	C9H20	69.2	9.2	prediction	255.3
C9_Mono-Naphthenes(23)		15505	propylcyclohexane	CCCC1CCCCC1	C9H18	69.2	2.1	experiment	160.9
C9_Mono-Naphthenes(24)		15505	propylcyclohexane	CCCC1CCCCC1	C9H18	69.2	2.1	experiment	160.9
Propylcyclohexane	1678-92-8	15505	propylcyclohexane	CCCC1CCCCC1	C9H18	69.2	2.1	experiment	145.4
5,5-Dimethyl-1,3-hexadiene	1515-79-3	5368952	(3E)-5,5-dimethylhexa-1,3-diene	CC(C)(C)C=CC=C	C8H14	69.6	11.8	prediction	367.8
n-Butylcyclopentane		16269	butylcyclopentane	CCCCC1CCCC1	C9H18	69.6	8.9	prediction	139.3
2t-Ethylmethylcyclopentane		12762848	(1S,2S)-1-ethyl-2-methylcyclopentane	CCC1CCCC1C	C8H16	69.6	9.3	prediction	312.4
3c-Ethylmethylcyclopentane	2613-66-3	19502	1-ethyl-3-methylcyclopentane	CCC1CCC(C1)C	C8H16	69.6	9.3	prediction	333.8
3t-Ethylmethylcyclopentane	3726-47-4	19502	1-ethyl-3-methylcyclopentane	CCC1CCC(C1)C	C8H16	69.6	9.3	prediction	333.8
C8_Mono-Naphthenes(4)		12762847	(1R,2S)-1-ethyl-2-methylcyclopentane	CCC1CCCC1C	C8H16	69.6	9.3	prediction	323.9
Cyclopentane, 1-ethyl-2-methyl	930-89-2	12762847	(1R,2S)-1-ethyl-2-methylcyclopentane	CCC1CCCC1C	C8H16	69.6	9.3	prediction	303.9
Cyclopentane, 1-ethyl-2-methyl-	3726-46-3	136729	1-ethyl-2-methylcyclopentane	CCC1CCCC1C	C8H16	69.6	9.3	prediction	302.8
Cyclopentane, 1-ethyl-2-methyl-cis		12762847	(1R,2S)-1-ethyl-2-methylcyclopentane	CCC1CCCC1C	C8H16	69.6	9.3	prediction	302.8
2,3-Dimethyloctane		23531	2,3-dimethyloctane	CCCCCC(C)C(C)C	C10H22	69.9	9.0	prediction	148.3
2,3-Dimethyloctane(1)		23531	2,3-dimethyloctane	CCCCCC(C)C(C)C	C10H22	69.9	9.0	prediction	115.8
2,4-Dimethyloctane		92978	2,4-dimethyloctane	CCCCC(C)CC(C)C	C10H22	69.9	9.0	prediction	140.5
2,5-Dimethyloctane	15869-89-3	139988	2,5-dimethyloctane	CCCC(C)CCC(C)C	C10H22	69.9	9.0	prediction	133.5
2,6-Dimethyloctane	2051-30-1	16319	2,6-dimethyloctane	CCC(C)CCCC(C)C	C10H22	69.9	9.0	prediction	129.6
2,7-dimethyloctane	1072-16-8	14070	2,7-dimethyloctane	CC(C)CCCCC(C)C	C10H22	69.9	9.0	prediction	133.5
3,6-Dimethyloctane		85927	3,6-dimethyloctane	CCC(C)CCC(C)CC	C10H22	69.9	9.0	prediction	126.2
3-Ethyl-2-methylheptane	14676-29-0	139803	3-ethyl-2-methylheptane	CCCCC(CC)C(C)C	C10H22	69.9	9.0	prediction	122.8
3-Methyl-5-ethylheptane	13475-78-0	26056	5-ethyl-2-methylheptane	CCC(CC)CCC(C)C	C10H22	69.9	9.0	prediction	130.6
C10_I-Paraffins(12)		16319	2,6-dimethyloctane	CCC(C)CCCC(C)C	C10H22	69.9	9.0	prediction	127.4
C10_I-Paraffins(13)		23531	2,3-dimethyloctane	CCCCCC(C)C(C)C	C10H22	69.9	9.0	prediction	118.9
C10_I-Paraffins(14)		23531	2,3-dimethyloctane	CCCCCC(C)C(C)C	C10H22	69.9	9.0	prediction	118.9
C10_I-Paraffins(15)		23531	2,3-dimethyloctane	CCCCCC(C)C(C)C	C10H22	69.9	9.0	prediction	115.8
C10_I-Paraffins(21)		139803	3-ethyl-2-methylheptane	CCCCC(CC)C(C)C	C10H22	69.9	9.0	prediction	30.0

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
Heptane, 3-ethyl-2-methyl-	14676-29-0	139803	3-ethyl-2-methylheptane	CCCCC(CC)C(C)C	C10H22	69.9	9.0	prediction	122.8
Octane, 3,4-dimethyl-	15869-92-8	85926	3,4-dimethyloctane	CCCCC(C)C(C)CC	C10H22	69.9	9.0	prediction	118.9
Cyclopentene	142-29-0	8882	cyclopentene	C1CC=CC1	C5H8	70.2	2.1	experiment	1,834.8
1c,2-Dimethylcyclohexane	112134	16628	(1S,2R)-1,2-dimethylcyclohexane	CC1CCCCC1C	C8H16	70.4	9.3	prediction	290.4
1t,2-Dimethylcyclohexane	6876-23-9	23313	(1R,2R)-1,2-dimethylcyclohexane	CC1CCCCC1C	C8H16	70.4	9.3	prediction	290.4
cis 1,2-dimethylcyclohexane	2207-01-4	16628	(1S,2R)-1,2-dimethylcyclohexane	CC1CCCCC1C	C8H16	70.4	9.3	prediction	290.4
Cyclohexane, 1,2-dimethyl-	583-57-3	11416	1,2-dimethylcyclohexane	CC1CCCCC1C	C8H16	70.4	9.3	prediction	290.4
2,3-dimethyl-2-pentene		25403	2,3-dimethylpent-2-ene	CCC(=C(C)C)C	C7H14	70.5	10.0	prediction	654.9
2,3-Dimethylpentene-2		25403	2,3-dimethylpent-2-ene	CCC(=C(C)C)C	C7H14	70.5	10.0	prediction	558.3
3-Ethylnonane		529886	3-ethylnonane	CCCCCCC(CC)CC	C11H24	70.7	8.9	prediction	83.3
3-Methyldecane		92239	3-methyldecane	CCCCCCCC(C)CC	C11H24	70.7	8.9	prediction	65.4
4-Methyldecane		17835	4-methyldecane	CCCCCCC(C)CCC	C11H24	70.7	8.9	prediction	93.6
5-Methyldecane		93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	71.9
C11_I-Paraffins(15)		93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(16)		93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(17)		93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(18)		93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(19)		23415	2-methyldecane	CCCCCCCCC(C)C	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(20)		23415	2-methyldecane	CCCCCCCCC(C)C	C11H24	70.7	8.9	prediction	65.5
C11_I-Paraffins(21)		92239	3-methyldecane	CCCCCCCC(C)CC	C11H24	70.7	8.9	prediction	70.6
C11_I-Paraffins(22)		92239	3-methyldecane	CCCCCCCC(C)CC	C11H24	70.7	8.9	prediction	70.6
Decane, 2-methyl-		23415	2-methyldecane	CCCCCCCCC(C)C	C11H24	70.7	8.9	prediction	83.3
Decane, 3-methyl-	13151-34-3	92239	3-methyldecane	CCCCCCCC(C)CC	C11H24	70.7	8.9	prediction	61.9
Decane, 4-methyl-	2847-72-5	17835	4-methyldecane	CCCCCCC(C)CCC	C11H24	70.7	8.9	prediction	64.7
Decane, 5-methyl-	13151-35-4	93071	5-methyldecane	CCCCCC(C)CCCC	C11H24	70.7	8.9	prediction	66.9
1,4-Hexadiene, 2-methyl-	1119-14-8	5367524	(4E)-2-methylhexa-1,4-diene	CC=CCC(=C)C	C7H12	71.5	9.3	prediction	703.8
3,3-Dimethylheptene-1		423787	3,3-dimethylhept-1-ene	CCCCC(C)(C)C=C	C9H18	71.6	9.2	prediction	250.0
t-2,2-Dimethylheptene-3		423787	3,3-dimethylhept-1-ene	CCCCC(C)(C)C=C	C9H18	71.6	9.2	prediction	269.7
3-Hexene, 2,2-dimethyl-, (E)-		5357261	(E)-2,2-dimethylhex-3-ene	CCC=CC(C)(C)C	C8H16	71.8	9.3	prediction	417.1
C13_I-Paraffins(2)		12388	tridecane	CCCCCCCCCCCCC	C13H28	72.5	3.6	experiment	17.5
n-Tridecane	629-50-5	12388	tridecane	CCCCCCCCCCCCC	C13H28	72.5	3.6	experiment	18.0
2,3,3-trimethyl-1-butene	594-56-9	11669	2,3,3-trimethylbut-1-ene	CC(=C)C(C)(C)C	C7H14	72.8	2.2	experiment	838.8
2,3,3-Trimethylbutene-1		11669	2,3,3-trimethylbut-1-ene	CC(=C)C(C)(C)C	C7H14	72.8	2.2	experiment	838.8
trans-2-Methyl-3-octene		5365951	(E)-2-methyloct-3-ene	CCCCC=CC(C)C	C9H18	73.3	9.1	prediction	206.9
3-Decene		5362724	(E)-dec-3-ene	CCCCCCC=CCC	C10H20	74.1	9.1	prediction	91.3
4-Decene		5364458	(E)-dec-4-ene	CCCCCC=CCCC	C10H20	74.1	9.1	prediction	131.2
trans-3-Decene		5362724	(E)-dec-3-ene	CCCCCCC=CCC	C10H20	74.1	9.1	prediction	103.0
trans-4-Decene	19398-89-1	5364458	(E)-dec-4-ene	CCCCCC=CCCC	C10H20	74.1	9.1	prediction	105.6
2,2,3,4-Tetramethylpentane	1186-53-4	14462	2,2,3,4-tetramethylpentane	CC(C)C(C)C(C)(C)C	C9H20	74.2	9.2	prediction	240.8
Pentane, 2,3,3,4-tetramethyl-	16747-38-9	28028	2,3,3,4-tetramethylpentane	CC(C)C(C)(C)C(C)C	C9H20	74.2	9.2	prediction	202.1
2,4-Dimethylheptene-1	19549-87-2	123385	2,4-dimethylhept-1-ene	CCCC(C)CC(=C)C	C9H18	74.7	9.2	prediction	222.2
2,6-Dimethylheptene-1	3074-78-0	76492	2,6-dimethylhept-1-ene	CC(C)CCCC(=C)C	C9H18	74.7	9.2	prediction	222.2
C9_Iso-Olefins(3)		123385	2,4-dimethylhept-1-ene	CCCC(C)CC(=C)C	C9H18	74.7	9.2	prediction	185.0
i-Propylcyclohexane		12763	propan-2-ylcyclohexane	CC(C)C1CCCCC1	C9H18	74.7	2.2	experiment	153.2
isopropylcyclohexane	696-29-7	12763	propan-2-ylcyclohexane	CC(C)C1CCCCC1	C9H18	74.7	2.2	experiment	156.7
C10_n-Olefins(1)		13381	dec-1-ene	CCCCCCCCC=C	C10H20	74.8	2.2	experiment	103.0
Decene-1		13381	dec-1-ene	CCCCCCCCC=C	C10H20	74.8	2.2	experiment	103.0
2,5-Dimethylhexene-2		18853	2,5-dimethylhex-2-ene	CC(C)CC=C(C)C	C8H16	74.8	9.1	prediction	344.8
2-Hexene, 2,4-dimethyl-	14255-23-3	518909	2,4-dimethylhex-2-ene	CCC(C)C=C(C)C	C8H16	74.8	9.1	prediction	413.4
2-Hexene, 2,5-dimethyl-	3404-78-2	18853	2,5-dimethylhex-2-ene	CC(C)CC=C(C)C	C8H16	74.8	9.1	prediction	379.8
2-Hexene, 3,5-dimethyl-	3404-79-3	5362848	(E)-3,5-dimethylhex-2-ene	CC=C(C)CC(C)C	C8H16	74.8	9.1	prediction	392.3
3,4-Dimethyl-t-2-hexene		5352662	(E)-3,4-dimethylhex-2-ene	CCC(C)C(=CC)C	C8H16	74.8	9.1	prediction	379.8
3,5-Dimethylhexene		640912	(Z)-3,5-dimethylhex-2-ene	CC=C(C)CC(C)C	C8H16	74.8	9.1	prediction	270.2

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
3-Hexene, 2,3-dimethyl-	7145-23-5	5357262	(E)-2,3-dimethylhex-3-ene	CCC=C(C)C(C)C	C8H16	74.8	9.1	prediction	379.8
1,1-Methylethylcyclopentane	16747-50-5	28030	1-ethyl-1-methylcyclopentane	CCC1(CCCC1)C	C8H16	74.9	11.4	prediction	342.4
2,2,4-trimethylheptane	14720-74-2	26839	2,2,4-trimethylheptane	CCCC(C)CC(C)(C)C	C10H22	75.0	9.0	prediction	167.3
3,3,5-TrimethylHeptane		23544	3,3,5-trimethylheptane	CCC(C)CC(C)(C)CC	C10H22	75.0	9.0	prediction	143.1
Heptane, 2,5,5-trimethyl-		14478	2,5,5-trimethylheptane	CCC(C)(C)CCC(C)C	C10H22	75.0	9.0	prediction	164.1
Heptane, 3,3,5-trimethyl-	7154-80-5	23544	3,3,5-trimethylheptane	CCC(C)CC(C)(C)CC	C10H22	75.0	9.0	prediction	142.6
i-Butylcyclopentane		77414	2-methylpropylcyclopentane	CC(C)CC1CCCC1	C9H18	75.4	9.0	prediction	163.3
3-Ethylcyclopentene	694-35-9	79095	3-ethylcyclopentene	CCC1CCC=C1	C7H12	75.4	9.6	prediction	553.3
2-Methyl-2-octene	16993-86-5	140163	2-methyloct-2-ene	CCCCCC=C(C)C	C9H18	75.6	9.1	prediction	176.3
2-Methyloctene-2	16993-86-4	140163	2-methyloct-2-ene	CCCCCC=C(C)C	C9H18	75.6	9.1	prediction	228.0
3-Heptene, 4-ethyl-	33933-74-3	5364679	(E)-4-ethylhept-3-ene	CCCC(=CCC)CC	C9H18	75.6	9.1	prediction	185.9
2,3,6-trimethylheptane		19944	2,3,6-trimethylheptane	CC(C)CCC(C)C(C)C	C10H22	75.8	9.2	prediction	138.8
C10_I-Paraffins(10)		19944	2,3,6-trimethylheptane	CC(C)CCC(C)C(C)C	C10H22	75.8	9.2	prediction	127.4
C10_I-Paraffins(11)		19944	2,3,6-trimethylheptane	CC(C)CCC(C)C(C)C	C10H22	75.8	9.2	prediction	127.4
C10_I-Paraffins(2)		140667	2,3,5-trimethylheptane	CCC(C)CC(C)C(C)C	C10H22	75.8	9.2	prediction	164.1
C10_I-Paraffins(3)		140667	2,3,5-trimethylheptane	CCC(C)CC(C)C(C)C	C10H22	75.8	9.2	prediction	138.8
C10_I-Paraffins(4)		140667	2,3,5-trimethylheptane	CCC(C)CC(C)C(C)C	C10H22	75.8	9.2	prediction	138.8
C10_I-Paraffins(7)		137658	2,4,6-trimethylheptane	CC(C)CC(C)CC(C)C	C10H22	75.8	9.2	prediction	127.4
C10_I-Paraffins(8)		19944	2,3,6-trimethylheptane	CC(C)CCC(C)C(C)C	C10H22	75.8	9.2	prediction	138.8
C10_I-Paraffins(9)		19944	2,3,6-trimethylheptane	CC(C)CCC(C)C(C)C	C10H22	75.8	9.2	prediction	127.4
Heptane, 2,3,5-trimethyl-	20278-85-7	140667	2,3,5-trimethylheptane	CCC(C)CC(C)C(C)C	C10H22	75.8	9.2	prediction	135.5
Heptane, 2,4,6-trimethyl-	2613-61-8	137658	2,4,6-trimethylheptane	CC(C)CC(C)CC(C)C	C10H22	75.8	9.2	prediction	168.1
1-Methyl-2-propyl-cyclopentan		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
C9_Mono-Naphthenes(13)		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
C9_Mono-Naphthenes(14)		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
C9_Mono-Naphthenes(15)		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
C9_Mono-Naphthenes(16)		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
C9_Mono-Naphthenes(17)		316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	156.7
Cyclopentane, 1-methyl-2-propyl	3728-57-2	316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	168.5
Cyclopentane, 1-methyl-2-propyl-	3728-57-2	316554	1-methyl-2-propylcyclopentane	CCCC1CCCC1C	C9H18	76.2	9.3	prediction	168.5
trans-1,2-Diethyl cyclopentane	932-40-1	6432778	(1R,2R)-1,2-diethylcyclopentane	CCC1CCCC1CC	C9H18	76.2	9.3	prediction	195.1
trans-1,3-Diethylcyclopentane		6537508	(1R,3R)-1,3-diethylcyclopentane	CCC1CCC(C1)CC	C9H18	76.2	9.3	prediction	187.7
1,2,4-Trimethylcyclopentane-A		17779	1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	325.2
1,2,4-Trimethylcyclopentane-B		17779	1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	324.6
1c,2c,3-Trimethylcyclopentane		35368	1,2,3-trimethylcyclopentane	CC1CCC(C1C)C	C8H16	76.2	10.3	prediction	352.4
1c,2c,4-Trimethylcyclopentane	2815-58-9	17779	1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	371.8
1c,2t,3-Trimethylcyclopentane	2613-69-6	35368	1,2,3-trimethylcyclopentane	CC1CCC(C1C)C	C8H16	76.2	10.3	prediction	362.4
1c,2t,4-Trimethylcyclopentane	4850-28-6	252323	(1R,2S)-1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	359.4
1t,2c,3-Trimethylcyclopentane	15890-40-1	27533	(1R,3R)-1,2,3-trimethylcyclopentane	CC1CCC(C1C)C	C8H16	76.2	10.3	prediction	362.7
Cyclopentane, 1,2,4-trimethyl-, (1à,2á,4à)-	16883-48-0	6429398	(1S,2S)-1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	362.7
Cyclopentane, 1,2,4-trimethyl-, (1α,2ß,4α)-		17779	1,2,4-trimethylcyclopentane	CC1CC(C(C1)C)C	C8H16	76.2	10.3	prediction	362.7
2,5-dimethylnonane		28456	2,5-dimethylnonane	CCCCC(C)CCC(C)C	C11H24	76.5	9.0	prediction	94.4
C11_I-Paraffins(24)		86541	4,5-dimethylnonane	CCCCC(C)C(C)CCC	C11H24	76.5	9.0	prediction	70.6
C11_I-Paraffins(25)		86541	4,5-dimethylnonane	CCCCC(C)C(C)CCC	C11H24	76.5	9.0	prediction	70.6
C11_I-Paraffins(4)		537768	6-ethyl-2-methyloctane	CCC(CC)CCCC(C)C	C11H24	76.5	9.0	prediction	78.9
C11_I-Paraffins(5)		537768	6-ethyl-2-methyloctane	CCC(CC)CCCC(C)C	C11H24	76.5	9.0	prediction	70.6
C11_I-Paraffins(6)		28456	2,5-dimethylnonane	CCCCC(C)CCC(C)C	C11H24	76.5	9.0	prediction	70.6
Nonane, 2,3-dimethyl-		520397	2,3-dimethylnonane	CCCCCCC(C)C(C)C	C11H24	76.5	9.0	prediction	65.5
Nonane, 2,5-dimethyl-		28456	2,5-dimethylnonane	CCCCC(C)CCC(C)C	C11H24	76.5	9.0	prediction	79.3
Nonane, 3,7-dimethyl-		28458	3,7-dimethylnonane	CCC(C)CCCC(C)CC	C11H24	76.5	9.0	prediction	71.8
Nonane, 4,5-dimethyl-		86541	4,5-dimethylnonane	CCCCC(C)C(C)CCC	C11H24	76.5	9.0	prediction	70.6
Octane, 5-ethyl-2-methyl-	62016-18-6	537332	5-ethyl-2-methyloctane	CCCC(CC)CCC(C)C	C11H24	76.5	9.0	prediction	81.8
Octane, 6-ethyl-2-methyl-	62016-19-7	537768	6-ethyl-2-methyloctane	CCC(CC)CCCC(C)C	C11H24	76.5	9.0	prediction	84.2

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
butylcyclohexane	1678-93-9	15506	butylcyclohexane	CCCCC1CCCCC1	C10H20	76.8	2.2	experiment	77.4
n-ButylCyclohexane	1678-93-9	15506	butylcyclohexane	CCCCC1CCCCC1	C10H20	76.8	2.2	experiment	77.4
1-Ethyl-3-methylcyclohexane (c,t)		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	161.9
1-ethyl-4-CIS-methylcyclohexane		19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	160.8
1-Ethyl-4-methylcyclohexane	3728-56-1	19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	160.9
1-ethyl-4-t-methylcyclohexane		19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	161.8
C9_Mono-Naphthenes(20)		19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	160.9
C9_Mono-Naphthenes(22)		19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	160.8
C9_Mono-Naphthenes(25)		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	184.1
C9_Mono-Naphthenes(26)		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	184.1
C9_Mono-Naphthenes(27)		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	155.6
C9_Mono-Naphthenes(28)		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	184.1
cis-1-Ethyl-3-methyl-cyclohexane	19489-10-2	29638	(1R,3S)-1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	160.9
Cyclohexane, 1-ethyl-2-methyl-		35413	1-ethyl-2-methylcyclohexane	CCC1CCCCC1C	C9H18	76.9	9.3	prediction	160.9
Cyclohexane, 1-ethyl-2-methyl-, cis-	4923-77-7	23620236	(1S,2R)-1-ethyl-2-methylcyclohexane	CCC1CCCCC1C	C9H18	76.9	9.3	prediction	141.9
Cyclohexane, 1-ethyl-3-methyl		35412	1-ethyl-3-methylcyclohexane	CCC1CCCC(C1)C	C9H18	76.9	9.3	prediction	168.7
Cyclohexane, 1-ethyl-4-methyl-		19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	168.7
Cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	19503	1-ethyl-4-methylcyclohexane	CCC1CCC(CC1)C	C9H18	76.9	9.3	prediction	160.9
2,3-Dimethyl-2-hexene	7145-20-2	23528	2,3-dimethylhex-2-ene	CCCC(=C(C)C)C	C8H16	77.1	10.0	prediction	317.9
3-Hexene, 3,4-dimethyl-, (Z)-		3034311	(Z)-3,4-dimethylhex-3-ene	CCC(=C(C)CC)C	C8H16	77.1	10.0	prediction	317.9
5-Ethyldecane		529848	5-ethyldecane	CCCCCC(CC)CCCC	C12H26	77.3	8.9	prediction	46.1
C12 - IsoParaffin - 1		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	45.5
C12 - IsoParaffin - 2		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	45.3
C12 - Isoparaffin - 3		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	37.7
C12 - IsoParaffin - 4		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	34.5
C12 - IsoParaffin - 6		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	38.3
C12_I-Paraffins(1)		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	70.6
C12_I-Paraffins(10)		519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	50.4
C12_I-Paraffins(11)		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	62.8
C12_I-Paraffins(2)		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	36.4
C12_I-Paraffins(3)		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	70.6
C12_I-Paraffins(7)		519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	46.1
C12_I-Paraffins(8)		519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	50.4
C12_I-Paraffins(9)		519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	50.4
C12-isoparaffin-1		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	63.0
C12-isoparaffin-7		519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	46.1
Decane, 4-ethyl-	1636-44-8	519256	4-ethyldecane	CCCCCCC(CC)CCC	C12H26	77.3	8.9	prediction	46.1
Undecane, 2-methyl-	7045-71-8	23459	2-methylundecane	CCCCCCCCCC(C)C	C12H26	77.3	8.9	prediction	36.7
Undecane, 4-methyl-		520454	4-methylundecane	CCCCCCCC(C)CCC	C12H26	77.3	8.9	prediction	36.4
2,3,3-Trimethylhexene-1		92984	3,5,5-trimethylhex-1-ene	CC(CC(C)(C)C)C=C	C9H18	77.4	9.2	prediction	270.1
3,5,5-Trimethylhexene-1		92984	3,5,5-trimethylhex-1-ene	CC(CC(C)(C)C)C=C	C9H18	77.4	9.2	prediction	282.4
C9 - IsoOlefin - 1		92984	3,5,5-trimethylhex-1-ene	CC(CC(C)(C)C)C=C	C9H18	77.4	9.2	prediction	258.4
C9 - Olefin - 1		92984	3,5,5-trimethylhex-1-ene	CC(CC(C)(C)C)C=C	C9H18	77.4	9.2	prediction	200.1
C14-Isoparaffin-1		12389	tetradecane	CCCCCCCCCCCCCC	C14H30	78.4	3.9	experiment	12.0
n-Tetradecane	629-59-4	12389	tetradecane	CCCCCCCCCCCCCC	C14H30	78.4	3.9	experiment	10.8
3,7-Dimethyloctene-1		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	141.2
C10 - IsoOlefin - 8		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	131.5
C10 Iso-olefin - 5		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	154.8
C10 Iso-olefin - 6		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	149.5
C10_Iso-Olefins(1)		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	176.3
C10_Iso-Olefins(2)		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	176.3
C10-IsoOlefin -15		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	105.0
C10-IsoOlefin-12		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	114.8

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
C10-IsoOlefin-4		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	156.2
C10-IsoOlefin-7		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	139.2
C10-n-Olefin		21085	3,7-dimethyloct-1-ene	CC(C)CCCC(C)C=C	C10H20	79.0	9.2	prediction	134.0
C8_Mono-Naphthenes(3)		15579940	(1S,2R)-1-butyl-2-methylcyclopropane	CCCCC1CC1C	C8H16	79.1	27.8	prediction	406.3
cis-1-Butyl-2-methylcyclopropane		15579940	(1S,2R)-1-butyl-2-methylcyclopropane	CCCCC1CC1C	C8H16	79.1	27.8	prediction	406.3
3-Heptene, 2,6-dimethyl-	2738-18-3	102326	2,6-dimethylhept-3-ene	CC(C)CC=CC(C)C	C9H18	79.2	9.3	prediction	234.6
2,3,3-Trimethyl-1-hexene	13427-43-5	530395	2,3,3-trimethylhex-1-ene	CCCC(C)(C)C(=C)C	C9H18	79.7	9.3	prediction	282.4
2,4,4-Trimethyl-1-hexene		142817	2,4,4-trimethylhex-1-ene	CCC(C)(C)CC(=C)C	C9H18	79.7	9.3	prediction	251.8
2-Pentene, 3,4,4-trimethyl-	39761-57-4	5357254	(E)-3,4,4-trimethylpent-2-ene	CC=C(C)C(C)(C)C	C8H16	79.8	9.3	prediction	431.0
2-Undecene, (E)-	693-61-8	5364452	(E)-undec-2-ene	CCCCCCCCC=CC	C11H22	80.7	9.1	prediction	74.1
5-Undecene		5364447	(E)-undec-5-ene	CCCCCC=CCCCC	C11H22	80.7	9.1	prediction	74.1
1-Octene, 2,6-dimethyl-	6874-29-9	522308	2,6-dimethyloct-1-ene	CCC(C)CCCC(=C)C	C10H20	81.2	9.2	prediction	159.5
2-Heptene, 2,6-dimethyl-		521663	2,6-dimethylhept-2-ene	CC(C)CCC=C(C)C	C9H18	81.4	9.1	prediction	230.4
3,5-Dimethyl-3-heptene	59643-68-4	5364776	(E)-3,5-dimethylhept-3-ene	CCC(C)C=C(C)CC	C9H18	81.4	9.1	prediction	230.4
2,3-Dimethyl-3-heptene	59643-74-2	5364739	(E)-2,3-dimethylhept-3-ene	CCCC=C(C)C(C)C	C9H18	81.4	9.4	prediction	184.6
1,1,2-Trimethylcyclopentane		35367	1,1,2-trimethylcyclopentane	CC1CCCC1(C)C	C8H16	81.5	11.2	prediction	407.8
1,1,3-Trimethylcyclopentane	4516-69-2	20615	1,1,3-trimethylcyclopentane	CC1CCC(C1)(C)C	C8H16	81.5	11.2	prediction	470.9
C8 - MonoNaph - 3		20615	1,1,3-trimethylcyclopentane	CC1CCC(C1)(C)C	C8H16	81.5	11.2	prediction	280.3
C8 MonoNaph - 1		20615	1,1,3-trimethylcyclopentane	CC1CCC(C1)(C)C	C8H16	81.5	11.2	prediction	337.8
C8 MonoNaph - 2		20615	1,1,3-trimethylcyclopentane	CC1CCC(C1)(C)C	C8H16	81.5	11.2	prediction	309.0
2,2,3-trimethyloctane	62016-26-6	188432	2,2,3-trimethyloctane	CCCCCC(C)C(C)(C)C	C11H24	81.5	9.0	prediction	78.9
2,2,6-Trimethyloctane	62016-28-8	522006	2,2,6-trimethyloctane	CCC(C)CCCC(C)(C)C	C11H24	81.5	9.0	prediction	94.9
2,3,3-trimethyloctane	62016-30-4	537321	2,3,3-trimethyloctane	CCCCCC(C)(C)C(C)C	C11H24	81.5	9.0	prediction	90.3
C11_I-Paraffins(2)		522006	2,2,6-trimethyloctane	CCC(C)CCCC(C)(C)C	C11H24	81.5	9.0	prediction	94.9
C11_I-Paraffins(3)		188432	2,2,3-trimethyloctane	CCCCCC(C)C(C)(C)C	C11H24	81.5	9.0	prediction	70.6
C11_I-Paraffins(7)		551285	2,6,6-trimethyloctane	CCC(C)(C)CCCC(C)C	C11H24	81.5	9.0	prediction	70.6
C11_I-Paraffins(8)		551285	2,6,6-trimethyloctane	CCC(C)(C)CCCC(C)C	C11H24	81.5	9.0	prediction	70.6
C11_I-Paraffins(9)		551285	2,6,6-trimethyloctane	CCC(C)(C)CCCC(C)C	C11H24	81.5	9.0	prediction	70.6
Octane, 2,2,6-trimethyl-		522006	2,2,6-trimethyloctane	CCC(C)CCCC(C)(C)C	C11H24	81.5	9.0	prediction	94.9
Octane, 2,3,3-trimethyl-	62016-30-2	537321	2,3,3-trimethyloctane	CCCCCC(C)(C)C(C)C	C11H24	81.5	9.0	prediction	90.3
Octane, 2,6,6-trimethyl-	54166-32-4	551285	2,6,6-trimethyloctane	CCC(C)(C)CCCC(C)C	C11H24	81.5	9.0	prediction	90.3
Cyclopentane, (1-methylbutyl)-	4737-43-3	521217	pentan-2-ylcyclopentane	CCCC(C)C1CCCC1	C10H20	82.0	9.0	prediction	93.0
Cyclopentane, (2-methylbutyl)-		521449	2-methylbutylcyclopentane	CCC(C)CC1CCCC1	C10H20	82.0	9.0	prediction	100.8
C9_Mono-Naphthenes(29)		521465	1-methyl-3-propan-2-ylcyclopentane	CC1CCC(C1)C(C)C	C9H18	82.0	9.4	prediction	197.1
Cyclopentane, 1-methyl-3-(1methylethyl)-		521465	1-methyl-3-propan-2-ylcyclopentane	CC1CCC(C1)C(C)C	C9H18	82.0	9.4	prediction	197.1
Cyclopentane, 1-methyl-3-(1-methylethyl)-	53771-88-3	521465	1-methyl-3-propan-2-ylcyclopentane	CC1CCC(C1)C(C)C	C9H18	82.0	9.4	prediction	197.1
3,5-Dimethylcyclopentene	7459-71-4	522549	3,5-dimethylcyclopentene	CC1CC(C=C1)C	C7H12	82.0	10.2	prediction	574.0
2-Nonene, 3-methyl-, (E)-		5366150	(E)-3-methylnon-2-ene	CCCCCCC(=CC)C	C10H20	82.2	9.1	prediction	131.6
3-Heptene, 4-propyl-	4485-13-6	138270	4-propylhept-3-ene	CCCC(=CCC)CCC	C10H20	82.2	9.1	prediction	127.1
3-Nonene, 3-methyl-, (E)-	69405-42-1	5364647	(E)-3-methylnon-3-ene	CCCCCC=C(C)CC	C10H20	82.2	9.1	prediction	131.6
3-Octene, 4-ethyl-	53966-51-1	521478	4-ethyloct-3-ene	CCCCC(=CCC)CC	C10H20	82.2	9.1	prediction	105.1
1,1-Methylethylcyclohexane	4926-90-3	35411	1-ethyl-1-methylcyclohexane	CCC1(CCCCC1)C	C9H18	82.2	11.4	prediction	155.6
2,4,6-Trimethyloctane	62016-37-9	545612	2,4,6-trimethyloctane	CCC(C)CC(C)CC(C)C	C11H24	82.3	9.3	prediction	95.1
2,5,6-Trimethyloctane	62016-14-2	545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	85.1
C11_I-Paraffins(10)		545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	79.3
C11_I-Paraffins(11)		545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	79.3
C11_I-Paraffins(12)		545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	70.6
C11_I-Paraffins(13)		545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	70.6
C11_I-Paraffins(14)		545571	2,5,6-trimethyloctane	CCC(C)C(C)CCC(C)C	C11H24	82.3	9.3	prediction	70.6
Octane, 2,3,6-trimethyl-		112465	2,3,6-trimethyloctane	CCC(C)CCC(C)C(C)C	C11H24	82.3	9.3	prediction	77.5
Octane, 2,3,7-trimethyl-	62016-34-6	43867	2,3,7-trimethyloctane	CC(C)CCCC(C)C(C)C	C11H24	82.3	9.3	prediction	79.5
C10_Mono-Naphthenes(9)		23468	butan-2-ylcyclohexane	CCC(C)C1CCCCC1	C10H20	82.7	9.1	prediction	79.5
i-Butylcyclohexane	1678-98-4	15508	2-methylpropylcyclohexane	CC(C)CC1CCCCC1	C10H20	82.7	9.1	prediction	97.3

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
sec-Butylcyclohexane		23468	butan-2-ylcyclohexane	CCC(C)C1CCCCC1	C10H20	82.7	9.1	prediction	79.5
C8_Naphtheno-Olefins(1)		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	258.9
C8_Naphtheno-Olefins(2)		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	258.9
C8_Naphtheno-Olefins(5)		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	271.6
C8_Naphtheno-Olefins(8)		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	253.1
C8-Napht-Olefin		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	382.6
Cyclohexene, 3-ethyl-		137724	3-ethylcyclohexene	CCC1CCCC=C1	C8H14	82.7	9.6	prediction	258.9
1c,2c,4c-Trimethylcyclohexane		91517	1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	192.5
1c,2c,4t-Trimethylcyclohexane		91517	1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	192.5
1c,2t,4t-Trimethylcyclohexane	7667-60-9	252327	(1S,2S,4S)-1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	194.1
C9_Mono-Naphthenes(11)		252327	(1S,2S,4S)-1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	187.7
C9_Mono-Naphthenes(12)		252327	(1S,2S,4S)-1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	234.6
Cyclohexane, 1,2,4-trimethyl-,		91517	1,2,4-trimethylcyclohexane	CC1CCC(C(C1)C)C	C9H18	82.8	2.4	experiment	196.9
2,3-Dimethyldecane		86544	2,3-dimethyldecane	CCCCCCCC(C)C(C)C	C12H26	83.1	9.0	prediction	37.6
2,6-Dimethyldecane		139395	2,6-dimethyldecane	CCCCC(C)CCCC(C)C	C12H26	83.1	9.0	prediction	45.7
C12_I-Paraffins(4)		519255	5,6-dimethyldecane	CCCCC(C)C(C)CCCC	C12H26	83.1	9.0	prediction	70.6
C12_I-Paraffins(5)		519255	5,6-dimethyldecane	CCCCC(C)C(C)CCCC	C12H26	83.1	9.0	prediction	70.6
Decane, 2,4-dimethyl-		520357	2,4-dimethyldecane	CCCCCCC(C)CC(C)C	C12H26	83.1	9.0	prediction	46.0
Decane, 2,5-dimethyl-	17312-50-4	519394	2,5-dimethyldecane	CCCCCC(C)CCC(C)C	C12H26	83.1	9.0	prediction	47.9
Decane, 3,7-dimethyl-		28468	3,7-dimethyldecane	CCCC(C)CCCC(C)CC	C12H26	83.1	9.0	prediction	43.0
Decane, 5,6-dimethyl-	1636-43-7	519255	5,6-dimethyldecane	CCCCC(C)C(C)CCCC	C12H26	83.1	9.0	prediction	41.7
C11 - MonoNaph - 1		20284	pentylcyclohexane	CCCCCC1CCCCC1	C11H22	83.5	9.0	prediction	85.9
C11 - MonoNaph - 2		20284	pentylcyclohexane	CCCCCC1CCCCC1	C11H22	83.5	9.0	prediction	59.9
C11 - MonoNaph - 3		20284	pentylcyclohexane	CCCCCC1CCCCC1	C11H22	83.5	9.0	prediction	46.9
C11_Mono-Naphthenes(1)		20284	pentylcyclohexane	CCCCCC1CCCCC1	C11H22	83.5	9.0	prediction	70.6
C11_Mono-Naphthenes(2)		20284	pentylcyclohexane	CCCCCC1CCCCC1	C11H22	83.5	9.0	prediction	70.6
1t-Methyl-2-n-propylcyclohexan		107252	1-methyl-2-propylcyclohexane	CCCC1CCCCC1C	C10H20	83.5	9.3	prediction	102.8
C10_Mono-Naphthenes(4)		14910	1,4-diethylcyclohexane	CCC1CCC(CC1)CC	C10H20	83.5	9.3	prediction	90.9
C10_Mono-Naphthenes(5)		14910	1,4-diethylcyclohexane	CCC1CCC(CC1)CC	C10H20	83.5	9.3	prediction	90.9
Diethylcylohexane		14910	1,4-diethylcyclohexane	CCC1CCC(CC1)CC	C10H20	83.5	9.3	prediction	136.1
Trans-1,4-diethylcyclohexane	13990-93-7	14910	1,4-diethylcyclohexane	CCC1CCC(CC1)CC	C10H20	83.5	9.3	prediction	90.9
1c,2t,4c-Trimethylcyclohexane	1795-26-2	35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	192.5
1c,3c,5-Trimethylcyclohexane	1839-63-0	35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	196.9
C9_Mono-Naphthenes(18)		35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	163.3
C9_Mono-Naphthenes(19)		35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	163.3
Cyclohexane, 1,2,3-trimethyl-, (1à,2à,3à)-	1839-88-9	6432164	(1R,3S)-1,2,3-trimethylcyclohexane	CC1CCCC(C1C)C	C9H18	83.6	10.2	prediction	168.5
Cyclohexane, 1,3,5-trimethyl-, (1à,3à,5á)-	1795-27-3	35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	210.9
Cyclohexane, 1,3,5-trimethyl-, (1α,3α,5ß)-		35364	1,3,5-trimethylcyclohexane	CC1CC(CC(C1)C)C	C9H18	83.6	10.2	prediction	210.9
2,3-Dimethylheptene-2		137816	2,3-dimethylhept-2-ene	CCCCC(=C(C)C)C	C9H18	83.6	10.0	prediction	184.6
C13_I-Paraffins(3)		519424	5-ethylundecane	CCCCCCC(CC)CCCC	C13H28	83.9	8.9	prediction	17.5
C13_I-Paraffins(4)		519397	3-ethylundecane	CCCCCCCCC(CC)CC	C13H28	83.9	8.9	prediction	25.4
Dodecane, 6-methyl-	6044-71-9	521926	6-methyldodecane	CCCCCCC(C)CCCCC	C13H28	83.9	8.9	prediction	23.7
Undecane, 3-ethyl-	17312-58-2	519397	3-ethylundecane	CCCCCCCCC(CC)CC	C13H28	83.9	8.9	prediction	20.8
Undecane, 5-ethyl-		519424	5-ethylundecane	CCCCCCC(CC)CCCC	C13H28	83.9	8.9	prediction	24.7
1,4-Hexadiene, 2,3-dimethyl-		5368910	(4E)-2,3-dimethylhexa-1,4-diene	CC=CC(C)C(=C)C	C8H14	83.9	9.4	prediction	381.5
n-Pentadecane	629-62-9	12391	pentadecane	CCCCCCCCCCCCCCC	C15H32	84.1	4.2	experiment	6.1
3-Hexyne, 2-methyl-		520802	2-methylhex-3-yne	CCC#CC(C)C	C7H12	84.1	11.4	prediction	562.1
Cyclohexene, 3-methyl-		11573	3-methylcyclohexene	CC1CCCC=C1	C7H12	85.0	4.0	experiment	477.4
C10 - MonoNaph - 2		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	105.7
C10 MonoNaphth - 3		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	104.0
C10_Mono-Naphthenes(1)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	97.3
C10_Mono-Naphthenes(10)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	143.3
C10_Mono-Naphthenes(11)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	166.3

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C10_Mono-Naphthenes(12)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	166.3
C10_Mono-Naphthenes(17)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	105.7
C10_Mono-Naphthenes(19)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	105.7
C10_Mono-Naphthenes(2)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	97.3
C10_Mono-Naphthenes(21)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	105.7
C10_Mono-Naphthenes(3)		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	81.2
C10-MonoNaph-2		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	105.7
C10-Naphthene-1		524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	97.3
Cyclooctane, 1,2-dimethyl-	13151-94-5	524411	1,2-dimethylcyclooctane	CC1CCCCCCC1C	C10H20	85.0	9.4	prediction	81.2
1,4-Pentadiene, 2,3,4-trimethy	72014-90-5	522437	2,3,4-trimethylpenta-1,4-diene	CC(C(=C)C)C(=C)C	C8H14	85.2	10.5	prediction	503.4
1,4-Pentadiene, 2,3,4-trimethyl-		522437	2,3,4-trimethylpenta-1,4-diene	CC(C(=C)C)C(=C)C	C8H14	85.2	10.5	prediction	503.4
4-Octene, 2,6-dimethyl-, [S-(Z)]-	62960-77-4	90474212	(E,6S)-2,6-dimethyloct-4-ene	CCC(C)C=CCC(C)C	C10H20	85.7	9.3	prediction	134.0
1-Undecene, 7-methyl-		522554	7-methylundec-1-ene	CCCCC(C)CCCCC=C	C12H24	86.3	9.1	prediction	40.7
2-Hexene, 2,5,5-trimethyl-		545914	2,5,5-trimethylhex-2-ene	CC(=CCC(C)(C)C)C	C9H18	86.4	9.3	prediction	239.6
C9_Iso-Olefins(1)		545914	2,5,5-trimethylhex-2-ene	CC(=CCC(C)(C)C)C	C9H18	86.4	9.3	prediction	239.6
C9-isoolefin		545914	2,5,5-trimethylhex-2-ene	CC(=CCC(C)(C)C)C	C9H18	86.4	9.3	prediction	195.3
C9-IsoOlefin-3		545914	2,5,5-trimethylhex-2-ene	CC(=CCC(C)(C)C)C	C9H18	86.4	9.3	prediction	209.2
1H-Indene, octahydro-, cis-	4551-51-3	643587	(3aS,7aR)-2,3,3a,4,5,6,7,7a-octahydro-1H-indene	C1CCC2CCCC2C1	C9H16	86.7	9.6	prediction	125.6
1H-Indene, octahydro-, trans-	3296-50-2	638055	(3aR,7aR)-2,3,3a,4,5,6,7,7a-octahydro-1H-indene	C1CCC2CCCC2C1	C9H16	86.7	9.6	prediction	125.6
Cyclopentene, 4,4-dimethyl-	19037-72-0	87906	4,4-dimethylcyclopentene	CC1(CC=CC1)C	C7H12	87.3	12.1	prediction	694.8
C11 - IsoParaffin - 10		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	30.8
C11 - IsoParaffin - 6		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	76.9
C11 - IsoParaffin - 9		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	67.4
C11- Isoparaffin - 12		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	66.5
C11- IsoParaffin - 13		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	61.4
C11 Isoparaffin - 4		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	91.5
C11 IsoParaffin - 5		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	87.7
C11 Isoparaffin-1		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	99.5
C11- Isoparaffin-10		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	68.3
C11- Isoparaffin-11		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	63.0
C11 Isoparaffin-2		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	97.5
C11 Isoparaffin-4		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	86.4
C11_I-Paraffins(1)		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	70.6
C11_I-Paraffins(26)		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	73.7
C11_I-Paraffins(27)		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	88.8
C11_I-Paraffins(28)		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	61.9
C11_I-Paraffins(29)		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	71.8
C11-Isoparaffin-1		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	112.5
C11-Isoparaffin-2		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	119.3
C11-Isoparaffin-3		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	96.2
C11-Isoparaffin-5		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	82.6
C11-Isoparaffin-7		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	76.1
C11-Isoparaffin-8		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	66.7
C11-Isoparaffin-9		545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	69.6
Heptane, 2,2,3,5-tetramethyl-	61868-42-6	545795	2,2,3,5-tetramethylheptane	CCC(C)CC(C)C(C)(C)C	C11H24	87.4	9.2	prediction	91.3
2-Octene, 3,7-dimethyl-, (Z)-		5352959	(E)-3,7-dimethyloct-2-ene	CC=C(C)CCCC(C)C	C10H20	88.0	9.1	prediction	133.0
hexadecane		11006	hexadecane	CCCCCCCCCCCCCCCC	C16H34	88.3	4.4	experiment	3.6
n-Hexadecane	544-76-3	11006	hexadecane	CCCCCCCCCCCCCCCC	C16H34	88.3	4.4	experiment	3.6
C10_Mono-Naphthenes(6)		21607535	1-methyl-3-(2-methylpropyl)cyclopentane	CC1CCC(C1)CC(C)C	C10H20	88.6	9.4	prediction	98.0
C10_Mono-Naphthenes(7)		21607535	1-methyl-3-(2-methylpropyl)cyclopentane	CC1CCC(C1)CC(C)C	C10H20	88.6	9.4	prediction	98.0
Cyclopentane, 1-methyl-3-(2methylpropyl)-		21607535	1-methyl-3-(2-methylpropyl)cyclopentane	CC1CCC(C1)CC(C)C	C10H20	88.6	9.4	prediction	166.3
Cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	520404	1-methyl-3-(2-methylpropyl)cyclopentane	CC1CCC(C1)CC(C)C	C10H20	88.6	9.4	prediction	166.3
1,1,2-Trimethylcyclohexane		35363	1,1,2-trimethylcyclohexane	CC1CCCCC1(C)C	C9H18	88.8	11.2	prediction	184.1

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
1,1,3-Trimethylcyclohexane		18309	1,1,3-trimethylcyclohexane	CC1CCCC(C1)(C)C	C9H18	88.8	11.2	prediction	216.0
1,1,4-Trimethylcyclohexane	7094-27-1	35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	234.6
C9_Mono-Naphthenes(10)		35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	234.6
C9_Mono-Naphthenes(21)		35363	1,1,2-trimethylcyclohexane	CC1CCCCC1(C)C	C9H18	88.8	11.2	prediction	160.9
C9_Mono-Naphthenes(5)		18309	1,1,3-trimethylcyclohexane	CC1CCCC(C1)(C)C	C9H18	88.8	11.2	prediction	234.6
C9_Mono-Naphthenes(6)		35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	196.9
C9_Mono-Naphthenes(7)		35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	234.6
C9_Mono-Naphthenes(8)		35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	234.6
C9_Mono-Naphthenes(9)		35365	1,1,4-trimethylcyclohexane	CC1CCC(CC1)(C)C	C9H18	88.8	11.2	prediction	234.6
Octane, 3-ethyl-2,7-dimethyl-	62183-55-5	537329	3-ethyl-2,7-dimethyloctane	CCC(CCCC(C)C)C(C)C	C12H26	88.9	9.3	prediction	47.2
2-pentyne,4,4-dimethyl		136786	4,4-dimethylpent-2-yne	CC#CC(C)(C)C	C7H12	89.2	11.5	prediction	772.1
2,4,4-trimethyl-2-pentene	107-40-4	7869	2,4,4-trimethylpent-2-ene	CC(=CC(C)(C)C)C	C8H16	89.3	2.6	experiment	480.7
C9 - NaphOlefin - 2		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	198.4
C9 Naph-Olefin -1		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	227.3
C9_Naphtheno-Olefins(1)		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	349.6
C9_Naphtheno-Olefins(2)		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	349.6
C9_Naphtheno-Olefins(3)		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	349.6
C9_Naphtheno-Olefins(4)		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	131.2
C9-NaphthenoOlefin-6		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	UNKN
Cyclohexene,3-propyl-		138092	3-propylcyclohexene	CCCC1CCCC=C1	C9H16	89.3	9.6	prediction	144.7
1-Isopropyl-3-MECY6	13837-67-7	13117022	(1R,3R)-1-methyl-3-propan-2-ylcyclohexane	CC1CCCC(C1)C(C)C	C10H20	89.3	9.4	prediction	101.8
C10_Mono-Naphthenes(8)		13117022	(1R,3R)-1-methyl-3-propan-2-ylcyclohexane	CC1CCCC(C1)C(C)C	C10H20	89.3	9.4	prediction	79.5
Cyclohexene, 3,5-dimethyl-		143321	3,5-dimethylcyclohexene	CC1CC=CC(C1)C	C8H14	89.4	10.1	prediction	308.3
trans-3,5-DimethylCyclohexene		12697641	(3R,5S)-3,5-dimethylcyclohexene	CC1CC=CC(C1)C	C8H14	89.4	10.1	prediction	314.3
1à,2á,3à,4á-Tetramethylcyclopentane	2532-67-4	137631	1,2,3,4-tetramethylcyclopentane	CC1CC(C(C1C)C)C	C9H18	89.4	11.7	prediction	234.6
1α,2ß,3α,4ß-Tetramethylcyclopentane		137631	1,2,3,4-tetramethylcyclopentane	CC1CC(C(C1C)C)C	C9H18	89.4	11.7	prediction	234.6
C13_I-Paraffins(5)		519384	2,8-dimethylundecane	CCCC(C)CCCCCC(C)C	C13H28	89.7	9.0	prediction	25.4
Undecane, 2,7-dimethyl-	17301-24-5	519383	2,7-dimethylundecane	CCCCC(C)CCCCC(C)C	C13H28	89.7	9.0	prediction	25.0
Undecane, 2,8-dimethyl-	17301-25-6	519384	2,8-dimethylundecane	CCCC(C)CCCCCC(C)C	C13H28	89.7	9.0	prediction	25.0
Cyclohexane, 1-ethyl-2,3-dimethyl-	1884043	550319	1-ethyl-2,3-dimethylcyclohexane	CCC1CCCC(C1C)C	C10H20	90.1	10.2	prediction	113.0
2,3-Dimethyl-2-octene		140599	2,3-dimethyloct-2-ene	CCCCCC(=C(C)C)C	C10H20	90.2	10.0	prediction	109.1
3-Ethyl-2-methylheptene-2		140589	3-ethyl-2-methylhept-2-ene	CCCCC(=C(C)C)CC	C10H20	90.2	10.0	prediction	100.2
cyclopentadiene		7612	cyclopenta-1,3-diene	C1C=CC=C1	C5H6	90.3	22.3	prediction	1,977.5
3-Heptyne, 5-methyl-		521962	5-methylhept-3-yne	CCC#CC(C)CC	C8H14	90.7	11.4	prediction	317.9
C8 - Diolefin - 1		521962	5-methylhept-3-yne	CCC#CC(C)CC	C8H14	90.7	11.4	prediction	374.0
C8 - Diolefin - 2		521962	5-methylhept-3-yne	CCC#CC(C)CC	C8H14	90.7	11.4	prediction	300.8
Cyclopropane, 1,1-diethyl-		66086	1,1-diethylcyclopropane	CCC1(CC1)CC	C7H14	91.7	37.3	prediction	691.7
Cyclohexane, 1-methyl-4-(1methylethyl)-, trans-			unknown	CC1CCC(CC1)C(C)C	C10H20	92.0	4.6	experiment	105.0
1,5-Heptadiene, 2,6-dimethyl-		81203	2,6-dimethylhepta-1,5-diene	CC(=CCCC(=C)C)C	C9H16	92.7	9.9	prediction	202.1
3-Hexene, 3-ethyl-2,5-dimethyl-	62338-08-3	543863	3-ethyl-2,5-dimethylhex-3-ene	CCC(=CC(C)C)C(C)C	C10H20	93.8	9.3	prediction	134.4
Heptane, 5-ethyl-2,2,3-trimethyl-	62199-06-8	545799	5-ethyl-2,2,3-trimethylheptane	CCC(CC)CC(C)C(C)(C)C	C12H26	93.9	9.2	prediction	50.8
Cyclohexane, 1-isopropyl-1-methyl-	16580-26-0	519284	1-methyl-1-propan-2-ylcyclohexane	CC(C)C1(CCCCC1)C	C10H20	94.6	11.5	prediction	118.1
C9 - MonoNaph - 1		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	244.9
C9 - MonoNaph - 2		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	221.6
C9 - MonoNaph - 2(1)		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	165.2
C9 - MonoNaph - 3		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	217.1
C9 - MonoNaph - 4		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	216.0
C9 - MonoNaph - 6		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	134.1
C9_Mono-Naphthenes(30)		6432224	(3S,4S)-1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	184.1
C9_Mono-Naphthenes(31)		6432224	(3S,4S)-1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	265.1
Cyclopentane, 1,1,3,4-tetramet		140671	1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	265.1
Cyclopentane, 1,1,3,4-tetramethyl-, trans-		6432224	(3S,4S)-1,1,3,4-tetramethylcyclopentane	CC1CC(CC1C)(C)C	C9H18	94.7	11.5	prediction	265.1
C12_I-Paraffins(6)		537765	2,3,6,7-tetramethyloctane	CC(C)C(C)CCC(C)C(C)C	C12H26	94.7	9.7	prediction	70.6

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Octane, 2,3,6,7-tetramethyl-		537765	2,3,6,7-tetramethyloctane	CC(C)C(C)CCC(C)C(C)C	C12H26	94.7	9.7	prediction	47.7
Cyclopentane, 1,2-dimethyl-3-(1methylethyl)-		544190	1,2-dimethyl-3-propan-2-ylcyclopentane	CC1CCC(C1C)C(C)C	C10H20	95.2	10.3	prediction	126.9
Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	544190	1,2-dimethyl-3-propan-2-ylcyclopentane	CC1CCC(C1C)C(C)C	C10H20	95.2	10.3	prediction	126.9
Cyclopentane, 2-isopropyl-1,3dimethyl-		543495	1,3-dimethyl-2-propan-2-ylcyclopentane	CC1CCC(C1C(C)C)C	C10H20	95.2	10.3	prediction	126.9
Cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	543495	1,3-dimethyl-2-propan-2-ylcyclopentane	CC1CCC(C1C(C)C)C	C10H20	95.2	10.3	prediction	126.9
C13 - IsoParaffin - 1		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	19.3
C13 - IsoParaffin - 2		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	17.4
C13 - IsoParaffin - 6		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	11.5
C13 - IsoParaffin - 7		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	10.2
C13_I-Paraffins(1)		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	17.5
C13_I-Paraffins(6)		522039	2,3,5-trimethyldecane	CCCCCC(C)CC(C)C(C)C	C13H28	95.5	9.3	prediction	20.8
C13_I-Paraffins(7)		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	64.1
C13_I-Paraffins(8)		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	70.6
C13_I-Paraffins(9)		545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	48.0
Decane, 2,3,4-trimethyl-		537769	2,3,4-trimethyldecane	CCCCCCC(C)C(C)C(C)C	C13H28	95.5	9.3	prediction	25.4
Decane, 2,3,5-trimethyl-		522039	2,3,5-trimethyldecane	CCCCCC(C)CC(C)C(C)C	C13H28	95.5	9.3	prediction	25.4
Decane, 2,3,6-trimethyl-		537330	2,3,6-trimethyldecane	CCCCC(C)CCC(C)C(C)C	C13H28	95.5	9.3	prediction	70.6
Decane, 2,3,8-trimethyl-	62238-14-6	545623	2,3,8-trimethyldecane	CCC(C)CCCCC(C)C(C)C	C13H28	95.5	9.3	prediction	25.4
Decane, 2,5,9-trimethyl-		522020	2,5,9-trimethyldecane	CC(C)CCCC(C)CCC(C)C	C13H28	95.5	9.3	prediction	34.6
Cyclobutane, 1-ethyl-3-methylene-		549131	1-ethyl-3-methylidenecyclobutane	CCC1CC(=C)C1	C7H12	95.7	11.0	prediction	568.8
t-2,2,5,5-Tetramethylhexene-3	692-47-7	5362849	(Z)-2,2,5,5-tetramethylhex-3-ene	CC(C)(C)C=CC(C)(C)C	C10H20	95.8	10.1	prediction	168.9
1-methyl-1-cyclopentene	693-89-0	12746	1-methylcyclopentene	CC1=CCCC1	C6H10	96.5	2.8	experiment	855.9
1-Methylcyclopentene		12746	1-methylcyclopentene	CC1=CCCC1	C6H10	96.5	2.8	experiment	855.9
C6_Naphtheno-Olefins(1)		12746	1-methylcyclopentene	CC1=CCCC1	C6H10	96.5	2.8	experiment	1,156.7
C6_Naphtheno-Olefins(2)		12746	1-methylcyclopentene	CC1=CCCC1	C6H10	96.5	2.8	experiment	1,156.7
C6_Naphtheno-Olefins(3)		12746	1-methylcyclopentene	CC1=CCCC1	C6H10	96.5	2.8	experiment	1,156.7
1,2,3,5-t-Tetramethylcyclohex		94276	1,2,3,5-tetramethylcyclohexane	CC1CC(C(C(C1)C)C)C	C10H20	96.7	11.6	prediction	127.4
1,6-Octadiene, 2,5-dimethyl-, (E)-		5362878	(6E)-2,5-dimethylocta-1,6-diene	CC=CC(C)CCC(=C)C	C10H18	97.0	9.4	prediction	144.2
3-Octyne, 6-methyl-	62108-34-3	534253	6-methyloct-3-yne	CCC#CCC(C)CC	C9H16	97.3	11.4	prediction	183.7
4-Octene, 2,3,6-trimethyl-		549902	2,3,6-trimethyloct-4-ene	CCC(C)C=CC(C)C(C)C	C11H22	98.1	9.7	prediction	86.5
1-Ethylcyclopentene	2146-38-5	137448	1-ethylcyclopentene	CCC1=CCCC1	C7H12	98.2	10.7	prediction	451.0
Heptane, 2,2,4,6,6-pentamethyl-		26058	2,2,4,6,6-pentamethylheptane	CC(CC(C)(C)C)CC(C)(C)C	C12H26	99.3	2.9	experiment	82.5
C9 MonoNaph - 3		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9_Mono-Naphthenes(1)		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9_Mono-Naphthenes(2)		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9_Mono-Naphthenes(3)		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9_Mono-Naphthenes(32)		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	141.9
C9_Mono-Naphthenes(4)		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	196.9
C9-MonoNaph-1		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9-MonoNaph-3		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	265.7
C9-MonoNaph-6		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	192.8
Cyclopentane, 1,1,3,3-tetramethyl-		123522	1,1,3,3-tetramethylcyclopentane	CC1(CCC(C1)(C)C)C	C9H18	99.9	16.9	prediction	348.8
2,4,6-Trimethyl-1-nonene		536118	2,4,6-trimethylnon-1-ene	CCCC(C)CC(C)CC(=C)C	C12H24	100.2	9.4	prediction	51.0
Benzene	71-42-3	241	benzene	C1=CC=CC=C1	C6H6	100.3	5.8	experiment	823.9
Cyclohexane, 1-methyl-4-(1methylethenyl)-, cis-		14299	1-methyl-4-prop-1-en-2-ylcyclohexane	CC1CCC(CC1)C(=C)C	C10H18	100.6	9.8	prediction	104.2
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-	1879-07-8	14299	1-methyl-4-prop-1-en-2-ylcyclohexane	CC1CCC(CC1)C(=C)C	C10H18	100.6	9.8	prediction	104.2
Cyclohexane, 1,1,3,5-tetramethyl-, trans-		55250338	(3S,5S)-1,1,3,5-tetramethylcyclohexane	CC1CC(CC(C1)(C)C)C	C10H20	102.0	11.5	prediction	140.7
2-Octene, 2,3,7-trimethyl-		557903	2,3,7-trimethyloct-2-ene	CC(C)CCCC(=C(C)C)C	C11H22	102.6	10.0	prediction	75.4
C11_Iso-Olefins(1)		557903	2,3,7-trimethyloct-2-ene	CC(C)CCCC(=C(C)C)C	C11H22	102.6	10.0	prediction	58.0
5-methyl-1,3cyclopentadiene		25512	5-methylcyclopenta-1,3-diene	CC1C=CC=C1	C6H8	103.5	22.5	prediction	974.3
Cyclobutane, (1-methylethylidene)-		519100	propan-2-ylidenecyclobutane	CC(=C1CCC1)C	C7H12	103.9	11.2	prediction	432.7
Cyclopentene, 1-propyl-		137815	1-propylcyclopentene	CCCC1=CCCC1	C8H14	104.8	10.7	prediction	247.1
Cyclopentene, 1,5-dimethyl-	16491-15-9	86014	1,5-dimethylcyclopentene	CC1CCC=C1C	C7H12	104.8	10.6	prediction	503.0

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
c-Decahydronaphthalene		7044	1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene	C1CCC2CCCCC2C1	C10H18	105.5	5.8	experiment	56.1
t-Decahydronaphthalene	493-02-7	7044	1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene	C1CCC2CCCCC2C1	C10H18	105.5	5.8	experiment	59.1
t-Decalin		7044	1,2,3,4,4a,5,6,7,8,8a-decahydronaphthalene	C1CCC2CCCCC2C1	C10H18	105.5	5.8	experiment	65.6
Cyclohexene, 1-ethyl-	1453-24-3	73937	1-ethylcyclohexene	CCC1=CCCCC1	C8H14	105.5	10.8	prediction	234.0
Heptane, 4-ethyl-2,2,6,6-tetramethyl-	62108-31-0	43925	4-ethyl-2,2,6,6-tetramethylheptane	CCC(CC(C)(C)C)CC(C)(C)C	C13H28	105.5	9.8	prediction	53.1
C13_Mono-Naphthenes(1)		21657239	1-ethyl-1-pentylcyclohexane	CCCCCC1(CCCCC1)CC	C13H26	108.5	11.5	prediction	40.7
C13-Mono-Naphthene-1		21657239	1-ethyl-1-pentylcyclohexane	CCCCCC1(CCCCC1)CC	C13H26	108.5	11.5	prediction	10.2
3-Heptyne, 5-ethyl-5-methyl-	61228-10-2	572963	5-ethyl-5-methylhept-3-yne	CCC#CC(C)(CC)CC	C10H18	108.9	11.5	prediction	144.3
3-Octyne, 2,2-dimethyl-		557206	2,2-dimethyloct-3-yne	CCCCC#CC(C)(C)C	C10H18	108.9	11.5	prediction	144.3
4-Octene, 2,2,3,7-tetramethyl-, [S-(E)]-		91693061	(E,3S)-2,2,3,7-tetramethyloct-4-ene	CC(C)CC=CC(C)C(C)(C)C	C12H24	109.7	9.6	prediction	45.5
4-Octene, 2,3,6,7-tetramethyl-	63830-66-0	549929	2,3,6,7-tetramethyloct-4-ene	CC(C)C(C)C=CC(C)C(C)C	C12H24	110.5	10.2	prediction	42.7
C12_Iso-Olefins(1)		549929	2,3,6,7-tetramethyloct-4-ene	CC(C)C(C)C=CC(C)C(C)C	C12H24	110.5	10.2	prediction	58.0
C12_Iso-Olefins(2)		549929	2,3,6,7-tetramethyloct-4-ene	CC(C)C(C)C=CC(C)C(C)C	C12H24	110.5	10.2	prediction	58.0
Cyclopentene, 1-(1-methylethyl)-		137017	1-propan-2-ylcyclopentene	CC(C)C1=CCCC1	C8H14	110.6	10.8	prediction	289.7
1-Ethyl-5-methylcyclopentene	97797-57-4	557171	1-ethyl-5-methylcyclopentene	CCC1=CCCC1C	C8H14	111.4	10.6	prediction	271.9
Cyclohexene,1-propyl-		107833	1-propylcyclohexene	CCCC1=CCCCC1	C9H16	112.1	10.8	prediction	131.2
1,3-Dimethyl-1-cyclohexene	2808-76-6	137726	1,3-dimethylcyclohexene	CC1CCCC(=C1)C	C8H14	112.1	10.6	prediction	285.0
1,4-Dimethyl-1-cyclohexene	70688-47-0	144440	1,4-dimethylcyclohexene	CC1CCC(=CC1)C	C8H14	112.1	10.6	prediction	285.0
C8 - Naph-Olefin - 1		137726	1,3-dimethylcyclohexene	CC1CCCC(=C1)C	C8H14	112.1	10.6	prediction	159.5
C8 - Naph-Olefin - 2		137726	1,3-dimethylcyclohexene	CC1CCCC(=C1)C	C8H14	112.1	10.6	prediction	150.3
C8 - Naph-Olefin - 5		137726	1,3-dimethylcyclohexene	CC1CCCC(=C1)C	C8H14	112.1	10.6	prediction	260.2
C8 Naph-Olefin - 6		137726	1,3-dimethylcyclohexene	CC1CCCC(=C1)C	C8H14	112.1	10.6	prediction	80.3
C8_Naphtheno-Olefins(3)		144440	1,4-dimethylcyclohexene	CC1CCC(=CC1)C	C8H14	112.1	10.6	prediction	349.6
trans-4a-Methyl-decahydronaphthalene		137634	8a-methyl-2,3,4,4a,5,6,7,8-octahydro-1H-naphthalene	CC12CCCCC1CCCC2	C11H20	112.5	11.6	prediction	49.4
4,7-Methano-1H-indene, octahydro-		17795	tricyclo[5.2.1.02,6]decane	C1CC2C3CCC(C3)C2C1	C10H16	114.7	11.4	prediction	89.0
Cyclohexane, butylidene-		549155	butylidenecyclohexane	CCCC=C1CCCCC1	C10H18	117.1	11.2	prediction	67.2
5-ethyl-1,3-dimethyl Indane		565493	1-ethyl-7a-methyl-1,2,3,3a,4,5,6,7-octahydroindene	CCC1CCC2C1(CCCC2)C	C12H22	124.9	11.4	prediction	9.1
Cyclopentane, 1,3-bis(methylene)-		556487	1,3-dimethylidenecyclopentane	C=C1CCC(=C)C1	C7H10	129.9	16.0	prediction	473.3
Cyclopropane, 1,2-dimethyl-1-pentyl-	62238-04-4	524630	1,2-dimethyl-1-pentylcyclopropane	CCCCCC1(CC1C)C	C10H20	130.0	18.9	prediction	137.3
1-Ethyl-2-Methylcyclopentene	1068-19-5	88243	1-ethyl-2-methylcyclopentene	CCC1=C(CCC1)C	C8H14	134.2	15.6	prediction	234.0
C8_Naphtheno-Olefins(4)		88243	1-ethyl-2-methylcyclopentene	CCC1=C(CCC1)C	C8H14	134.2	15.6	prediction	349.6
Methyl ethyl cyclopentene		88243	1-ethyl-2-methylcyclopentene	CCC1=C(CCC1)C	C8H14	134.2	15.6	prediction	272.6
1,2,3-Trimethylcyclopentene		136316	1,2,3-trimethylcyclopentene	CC1CCC(=C1C)C	C8H14	140.8	15.5	prediction	318.3
Cyclopentene, 1,2,3-trimethyl-	473-91-6	136316	1,2,3-trimethylcyclopentene	CC1CCC(=C1C)C	C8H14	140.8	15.5	prediction	329.9
1,3-Cyclopentadiene, 1,2-dimet		0	unknown	CC1=C(C=CC1)C	C7H10	147.3	23.9	prediction	455.1
Toluene	108-88-3	1140	toluene	CC1=CC=CC=C1	C7H8	170.9	7.7	experiment	413.4
1,4-Cyclohexadiene, 1-methyl-		78006	1-methylcyclohexa-1,4-diene	CC1=CCC=CC1	C7H10	175.6	7.7	experiment	404.1
1-methyl-1,4-cyclohexadiene	4313-57-9	78006	1-methylcyclohexa-1,4-diene	CC1=CCC=CC1	C7H10	175.6	7.7	experiment	404.1
i-Propylbenzene		7406	cumene	CC(C)C1=CC=CC=C1	C9H12	187.6	8.2	experiment	154.8
isopropylbenzene	98-82-8	7406	cumene	CC(C)C1=CC=CC=C1	C9H12	187.6	8.2	experiment	154.8
(1-methylpropyl)-benzene	135-98-8	8680	butan-2-ylbenzene	CCC(C)C1=CC=CC=C1	C10H14	199.1	8.7	experiment	92.5
sec-Butylbenzene		8680	butan-2-ylbenzene	CCC(C)C1=CC=CC=C1	C10H14	199.1	8.7	experiment	92.5
1,2-dimethylbenzene	95-47-6	7237	1,2-xylene	CC1=CC=CC=C1C	C8H10	200.0	10.0	experiment	194.1
o-Xylene		7237	1,2-xylene	CC1=CC=CC=C1C	C8H10	200.0	10.0	experiment	194.1
1,4-dimethylbenzene	106-42-3	7809	1,4-xylene	CC1=CC=C(C=C1)C	C8H10	202.0	10.1	experiment	210.4
p-Xylene		7809	1,4-xylene	CC1=CC=C(C=C1)C	C8H10	202.0	10.1	experiment	210.4
Ethylbenzene	100-41-4	7500	ethylbenzene	CCC1=CC=CC=C1	C8H10	216.0	10.8	experiment	228.0
1,3-dimethylbenzene	108-38-3	7929	1,3-xylene	CC1=CC(=CC=C1)C	C8H10	221.6	9.3	experiment	218.5
m-Xylene		7929	1,3-xylene	CC1=CC(=CC=C1)C	C8H10	221.6	9.3	experiment	218.5
1-Methyl-1-n-butylbenzene		17627	pentan-2-ylbenzene	CCCC(C)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	56.1
Benzene, (1-ethylpropyl)-		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	64.5
Benzene, (1-methylbutyl)-	2719-52-0	17627	pentan-2-ylbenzene	CCCC(C)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	41.6
C11 - Aromatic - 1		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	49.7

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
C11 - Aromatic - 10		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	37.7
C11 - Aromatic - 11		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	29.1
C11 - Aromatic - 12		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	27.6
C11 - Aromatic - 13		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	25.9
C11 - Aromatic - 14		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	25.4
C11 - Aromatic - 2		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	48.4
C11 - Aromatic - 3		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	43.1
C11 - Aromatic - 4		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	40.6
C11 - Aromatic - 6		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	43.2
C11 - Aromatic - 7		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	35.6
C11_Mono-Aromatics(1)		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	66.5
C11_Mono-Aromatics(15)		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	32.8
C11_Mono-Aromatics(16)		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	32.8
C11-Aromatic-14		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	26.0
C11-Aromatic-15		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	23.5
C11-Aromatic-9		14527	pentan-3-ylbenzene	CCC(CC)C1=CC=CC=C1	C11H16	230.4	13.6	prediction	34.7
n-Propylbenzene		7668	propylbenzene	CCCC1=CC=CC=C1	C9H12	235.7	9.9	experiment	127.1
propylbenzene	103-65-1	7668	propylbenzene	CCCC1=CC=CC=C1	C9H12	235.7	9.9	experiment	127.1
(1,2-dimethylpropyl)benzene	4481-30-5	98361	3-methylbutan-2-ylbenzene	CC(C)C(C)C1=CC=CC=C1	C11H16	236.2	13.6	prediction	66.5
Benzene, (1-methylpentyl)-		22385	hexan-2-ylbenzene	CCCCC(C)C1=CC=CC=C1	C12H18	237.0	13.6	prediction	37.6
Benzene, (1,3-dimethylbutyl)-	19219-84-2	519646	4-methylpentan-2-ylbenzene	CC(C)CC(C)C1=CC=CC=C1	C12H18	242.8	13.6	prediction	37.9
n-Butylbenzene	104-51-8	7705	butylbenzene	CCCCC1=CC=CC=C1	C10H14	245.1	9.9	experiment	71.8
n-Hexylbenzene	1077-16-3	14109	hexylbenzene	CCCCCCC1=CC=CC=C1	C12H18	246.7	9.9	experiment	22.9
Benzene, (2-ethylbutyl)-		29509	2-ethylbutylbenzene	CCC(CC)CC1=CC=CC=C1	C12H18	251.2	9.7	prediction	28.5
C12_Mono-Aromatics(9)		29509	2-ethylbutylbenzene	CCC(CC)CC1=CC=CC=C1	C12H18	251.2	9.7	prediction	37.6
n-Pentylbenzene	538-68-1	10864	pentylbenzene	CCCCCC1=CC=CC=C1	C11H16	255.0	10.5	experiment	40.3
s-Pentylbenzene		10864	pentylbenzene	CCCCCC1=CC=CC=C1	C11H16	255.0	10.5	experiment	38.0
Benzene, (3,3-dimethylbutyl)-		519406	3,3-dimethylbutylbenzene	CC(C)(C)CCC1=CC=CC=C1	C12H18	256.2	9.8	prediction	24.1
C12_Mono-Aromatics(4)		519406	3,3-dimethylbutylbenzene	CC(C)(C)CCC1=CC=CC=C1	C12H18	256.2	9.8	prediction	37.9
1-ethyl-4-methylbenzene	622-96-8	12160	1-ethyl-4-methylbenzene	CCC1=CC=C(C=C1)C	C9H12	257.1	10.5	experiment	122.5
1-Methyl-4-ethylbenzene		12160	1-ethyl-4-methylbenzene	CCC1=CC=C(C=C1)C	C9H12	257.1	10.5	experiment	122.5
(2-methylpropyl)-benzene	538-93-2	10870	2-methylpropylbenzene	CC(C)CC1=CC=CC=C1	C10H14	257.6	10.5	experiment	87.8
i-Butylbenzene		10870	2-methylpropylbenzene	CC(C)CC1=CC=CC=C1	C10H14	257.6	10.5	experiment	87.8
Isopentyl benzene		16294	3-methylbutylbenzene	CC(C)CCC1=CC=CC=C1	C11H16	258.1	10.5	experiment	54.7
Benzene, (2,4-dimethylpentyl)-	54518-00-2	143178	2,4-dimethylpentylbenzene	CC(C)CC(C)CC1=CC=CC=C1	C13H20	263.6	9.9	prediction	18.9
1-ethyl-2-methylbenzene	611-14-3	11903	1-ethyl-2-methylbenzene	CCC1=CC=CC=C1C	C9H12	267.0	11.0	experiment	116.6
1-Methyl-2-ethylbenzene		11903	1-ethyl-2-methylbenzene	CCC1=CC=CC=C1C	C9H12	267.0	11.0	experiment	116.6
1,4-Diethylbenzene	105-05-5	7734	1,4-diethylbenzene	CCC1=CC=C(C=C1)CC	C10H14	270.7	11.0	experiment	92.5
1-ethyl-3-methylbenzene	620-14-4	12100	1-ethyl-3-methylbenzene	CCC1=CC=CC(=C1)C	C9H12	278.0	11.1	experiment	124.6
1-Methyl-3-ethylbenzene		12100	1-ethyl-3-methylbenzene	CCC1=CC=CC(=C1)C	C9H12	278.0	11.1	experiment	124.6
1-Methyl-3-i-propylbenzene	535-77-3	10812	1-methyl-3-propan-2-ylbenzene	CC1=CC(=CC=C1)C(C)C	C10H14	278.6	13.5	prediction	88.4
1-methyl-4-(1-methylpropyl)be	1595-16-0	519195	1-butan-2-yl-4-methylbenzene	CCC(C)C1=CC=C(C=C1)C	C11H16	285.1	13.5	prediction	51.8
1-Methyl-2-i-propylbenzene	1074-17-5	14091	1-methyl-2-propylbenzene	CCCC1=CC=CC=C1C	C10H14	286.9	9.7	prediction	81.8
1-Methyl-2-n-propylbenzene	1074-17-5	14091	1-methyl-2-propylbenzene	CCCC1=CC=CC=C1C	C10H14	286.9	9.7	prediction	66.2
1-Methyl-3-n-propylbenzene	1074-43-7	14092	1-methyl-3-propylbenzene	CCCC1=CC=CC(=C1)C	C10H14	286.9	9.7	prediction	71.1
1-Methyl-4-i-propylbenzene		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	86.5
1-Methyl-4-n-propylbenzene	1074-55-1	14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	70.2
C10_Mono-Aromatics(1)		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	88.4
C10_Mono-Aromatics(10)		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	71.5
C10_Mono-Aromatics(11)		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	66.2
C10_Mono-Aromatics(8)		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	87.8
C10_Mono-Aromatics(9)		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	65.3
C10-Aromatic-0		14095	1-methyl-4-propylbenzene	CCCC1=CC=C(C=C1)C	C10H14	286.9	9.7	prediction	88.4

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
(1,1-dimethylethyl)-benzene	98-06-6	7366	tert-butylbenzene	CC(C)(C)C1=CC=CC=C1	C10H14	291.1	11.6	experiment	106.2
t-Butylbenzene		7366	tert-butylbenzene	CC(C)(C)C1=CC=CC=C1	C10H14	291.1	11.6	experiment	106.2
1-Methyl-2-n-butylbenzene	577-55-9	62410	1-butyl-2-methylbenzene	CCCCC1=CC=CC=C1C	C11H16	293.5	9.7	prediction	41.8
1-Methyl-3-n-butylbenzene		15327	1-butyl-3-methylbenzene	CCCCC1=CC=CC(=C1)C	C11H16	293.5	9.7	prediction	40.7
4M-1tC4Benz		15328	1-butyl-4-methylbenzene	CCCCC1=CC=C(C=C1)C	C11H16	293.5	9.7	prediction	59.1
C11_Mono-Aromatics(8)		62410	1-butyl-2-methylbenzene	CCCCC1=CC=CC=C1C	C11H16	293.5	9.7	prediction	35.6
Benzene, (1,1-dimethylpropyl)-		16295	2-methylbutan-2-ylbenzene	CCC(C)(C)C1=CC=CC=C1	C11H16	297.7	17.3	prediction	60.5
tert-pentyl benzene		16295	2-methylbutan-2-ylbenzene	CCC(C)(C)C1=CC=CC=C1	C11H16	297.7	17.3	prediction	44.9
tert-Pentylbenzene	2049-95-8	16295	2-methylbutan-2-ylbenzene	CCC(C)(C)C1=CC=CC=C1	C11H16	297.7	17.3	prediction	60.5
Benzene, 1-methyl-4-(2-methylpropyl)	1191153	21240	1-methyl-4-(2-methylpropyl)benzene	CC1=CC=C(C=C1)CC(C)C	C11H16	299.3	9.8	prediction	36.4
Benzene, 1-methyl-4-(2-methylpropyl)-	5161-04-6	21240	1-methyl-4-(2-methylpropyl)benzene	CC1=CC=C(C=C1)CC(C)C	C11H16	299.3	9.8	prediction	51.7
C11_Mono-Aromatics(2)		21240	1-methyl-4-(2-methylpropyl)benzene	CC1=CC=C(C=C1)CC(C)C	C11H16	299.3	9.8	prediction	60.0
1-Methyl-4-n-pentylbenzene		524159	1-methyl-4-pentylbenzene	CCCCCC1=CC=C(C=C1)C	C12H18	300.1	9.7	prediction	22.5
C12_Mono-Aromatics(5)		524159	1-methyl-4-pentylbenzene	CCCCCC1=CC=C(C=C1)C	C12H18	300.1	9.7	prediction	41.8
C12_Mono-Aromatics(6)		524159	1-methyl-4-pentylbenzene	CCCCCC1=CC=C(C=C1)C	C12H18	300.1	9.7	prediction	41.8
Benzene, (1,1-dimethylbutyl)-		16136	2-methylpentan-2-ylbenzene	CCCC(C)(C)C1=CC=CC=C1	C12H18	304.3	17.3	prediction	40.2
Benzene, (1-ethyl-1-methylpropyl)-		583611	3-methylpentan-3-ylbenzene	CCC(C)(CC)C1=CC=CC=C1	C12H18	304.3	17.3	prediction	40.7
1-methyl-2-N-hexylbenzene		524663	1-hexyl-2-methylbenzene	CCCCCCC1=CC=CC=C1C	C13H20	306.7	9.7	prediction	18.3
1-Methyl-3-hexyl benzene		571731	1-hexyl-3-methylbenzene	CCCCCCC1=CC=CC(=C1)C	C13H20	306.7	9.7	prediction	9.7
1-Methyl-3-Hexylbenzene		571731	1-hexyl-3-methylbenzene	CCCCCCC1=CC=CC(=C1)C	C13H20	306.7	9.7	prediction	9.7
1-Methyl-4-Hexylbenzene	1595-01-3	519194	1-hexyl-4-methylbenzene	CCCCCCC1=CC=C(C=C1)C	C13H20	306.7	9.7	prediction	13.0
C13 - Aromatic - 2		519194	1-hexyl-4-methylbenzene	CCCCCCC1=CC=C(C=C1)C	C13H20	306.7	9.7	prediction	21.6
C13-Aromatic-2		519194	1-hexyl-4-methylbenzene	CCCCCCC1=CC=C(C=C1)C	C13H20	306.7	9.7	prediction	12.3
C13-Aromatic-3		519194	1-hexyl-4-methylbenzene	CCCCCCC1=CC=C(C=C1)C	C13H20	306.7	9.7	prediction	10.0
C13-Aromatic-4		519194	1-hexyl-4-methylbenzene	CCCCCCC1=CC=C(C=C1)C	C13H20	306.7	9.7	prediction	9.9
1,2-Di-i-propylbenzene		11345	1,2-di(propan-2-yl)benzene	CC(C)C1=CC=CC=C1C(C)C	C12H18	307.7	22.3	prediction	42.0
1,4-Di-i-propylbenzene	100-18-5	7486	1,4-di(propan-2-yl)benzene	CC(C)C1=CC=C(C=C1)C(C)C	C12H18	307.7	22.3	prediction	35.3
1,2,4-Trimethylbenzene	95-63-6	7247	1,2,4-trimethylbenzene	CC1=CC(=C(C=C1)C)C	C9H12	308.3	12.2	experiment	105.6
1-Ethyl-3-i-propylbenzene		21030	1-ethyl-3-propan-2-ylbenzene	CCC1=CC(=CC=C1)C(C)C	C11H16	309.5	14.1	prediction	42.7
1-Ethyl-4-i-propylbenzene	4218-48-8	20197	1-ethyl-4-propan-2-ylbenzene	CCC1=CC=C(C=C1)C(C)C	C11H16	309.5	14.1	prediction	50.4
Benzene, 1-ethyl-3-(1-methylethyl)-	4920-99-4	21030	1-ethyl-3-propan-2-ylbenzene	CCC1=CC(=CC=C1)C(C)C	C11H16	309.5	14.1	prediction	56.7
Benzene, (1,1,2-trimethylpropyl)-		520256	2,3-dimethylbutan-2-ylbenzene	CC(C)C(C)(C)C1=CC=CC=C1	C12H18	310.1	17.3	prediction	24.4
Benzene, 2-propenyl-		9309	prop-2-enylbenzene	C=CCC1=CC=CC=C1	C9H10	310.9	12.3	experiment	106.9
1,3,5-Trimethylbenzene	108-67-8	0	1,3,5-trimethylbenzene	CC1=CC(=CC(=C1)C)C	C9H12	310.9	12.3	experiment	109.1
1,2,3-Trimethylbenzene	526-73-8	10686	1,2,3-trimethylbenzene	CC1=C(C(=CC=C1)C)C	C9H12	315.1	12.3	experiment	88.7
C9_Mono-Aromatics(1)		10686	1,2,3-trimethylbenzene	CC1=C(C(=CC=C1)C)C	C9H12	315.1	12.3	experiment	86.2
1-Ethyl-2-i-propylbenzene		519210	1-ethyl-2-propylbenzene	CCCC1=CC=CC=C1CC	C11H16	317.9	12.0	prediction	42.7
1-Ethyl-2-n-propylbenzene		519210	1-ethyl-2-propylbenzene	CCCC1=CC=CC=C1CC	C11H16	317.9	12.0	prediction	56.1
1,3-Diethylbenzene	141-93-5	8864	1,3-diethylbenzene	CCC1=CC(=CC=C1)CC	C10H14	320.9	12.8	experiment	74.8
1,3-Di-n-propylbenzene		519365	1,3-dipropylbenzene	CCCC1=CC(=CC=C1)CCC	C12H18	324.4	11.9	prediction	43.0
Benzene, 1-ethyl-4-(2-methylpropyl)-	100319-40-2	576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	19.3
C12 - Aromatic - 1		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	23.4
C12 - Aromatic - 10		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	23.3
C12 - Aromatic - 11		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	16.0
C12 - Aromatic - 11(1)		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	16.0
C12 - Aromatic - 2		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	23.0
C12 - Aromatic - 3		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	22.5
C12 - Aromatic - 4		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	23.0
C12 - Aromatic - 5		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	22.5
C12 - Aromatic - 7		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	20.8
C12 - Aromatic -8		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	20.4
C12_Mono-Aromatics(1)		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	41.8
C12_Mono-Aromatics(18)		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	40.7

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
C12-Aromatic-1		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	32.8
C12-Aromatic-8		576929	1-ethyl-4-(2-methylpropyl)benzene	CCC1=CC=C(C=C1)CC(C)C	C12H18	330.3	12.0	prediction	11.1
1-isopropyl-4-methylbenzene	99-87-6	7463	1-methyl-4-propan-2-ylbenzene	CC1=CC=C(C=C1)C(C)C	C10H14	330.3	12.9	experiment	86.5
Naphthalene, 1,2,3,4-tetrahydro		8404	1,2,3,4-tetrahydronaphthalene	C1CCC2=CC=CC=C2C1	C10H12	336.0	13.4	experiment	35.3
Benzene, 1,3-dimethyl-5-(1methylethyl)-		20833	1,3-dimethyl-5-propan-2-ylbenzene	CC1=CC(=CC(=C1)C(C)C)C	C11H16	339.9	14.0	prediction	54.6
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	4706-90-5	20833	1,3-dimethyl-5-propan-2-ylbenzene	CC1=CC(=CC(=C1)C(C)C)C	C11H16	339.9	14.0	prediction	54.6
Benzene, 1,4-dimethyl-2-(1methylethyl)-		77784	1,4-dimethyl-2-propan-2-ylbenzene	CC1=CC(=C(C=C1)C)C(C)C	C11H16	339.9	14.0	prediction	51.4
Benzene, 1,4-dimethyl-2-(1-methylethyl)-	4132-72-3	77784	1,4-dimethyl-2-propan-2-ylbenzene	CC1=CC(=C(C=C1)C)C(C)C	C11H16	339.9	14.0	prediction	51.4
Benzene, 2,4-dimethyl-1-(1methylethyl)-		20832	2,4-dimethyl-1-propan-2-ylbenzene	CC1=CC(=C(C=C1)C(C)C)C	C11H16	339.9	14.0	prediction	47.3
Benzene, 2,4-dimethyl-1-(1-methylethyl)-	4706-89-2	20832	2,4-dimethyl-1-propan-2-ylbenzene	CC1=CC(=C(C=C1)C(C)C)C	C11H16	339.9	14.0	prediction	47.3
C11_Mono-Aromatics(12)		20832	2,4-dimethyl-1-propan-2-ylbenzene	CC1=CC(=C(C=C1)C(C)C)C	C11H16	339.9	14.0	prediction	56.2
C11_Mono-Aromatics(13)		20832	2,4-dimethyl-1-propan-2-ylbenzene	CC1=CC(=C(C=C1)C(C)C)C	C11H16	339.9	14.0	prediction	56.2
C11_Mono-Aromatics(14)		20832	2,4-dimethyl-1-propan-2-ylbenzene	CC1=CC(=C(C=C1)C(C)C)C	C11H16	339.9	14.0	prediction	56.2
1,2-Dimethyl-3-ethylbenzene	933-98-2	13621	1-ethyl-2,3-dimethylbenzene	CCC1=CC=CC(=C1C)C	C10H14	341.6	10.7	prediction	57.4
1,2-Dimethyl-4-ethylbenzene	934-80-5	13629	4-ethyl-1,2-dimethylbenzene	CCC1=CC(=C(C=C1)C)C	C10H14	341.6	10.7	prediction	61.2
1,3-Dimethyl-2-ethylbenzene	2870-04-4	17877	2-ethyl-1,3-dimethylbenzene	CCC1=C(C=CC=C1C)C	C10H14	341.6	10.7	prediction	60.3
1,3-Dimethyl-4-ethylbenzene	874-41-9	13403	1-ethyl-2,4-dimethylbenzene	CCC1=C(C=C(C=C1)C)C	C10H14	341.6	10.7	prediction	63.8
1,3-Dimethyl-5-ethylbenzene	934-74-7	13627	1-ethyl-3,5-dimethylbenzene	CCC1=CC(=CC(=C1)C)C	C10H14	341.6	10.7	prediction	69.5
1,4,Dimethyl-2-ethylbenzene	1758-88-9	15653	2-ethyl-1,4-dimethylbenzene	CCC1=C(C=CC(=C1)C)C	C10H14	341.6	10.7	prediction	65.5
C10_Mono-Aromatics(4)		13403	1-ethyl-2,4-dimethylbenzene	CCC1=C(C=C(C=C1)C)C	C10H14	341.6	10.7	prediction	65.5
C10_Mono-Aromatics(5)		13403	1-ethyl-2,4-dimethylbenzene	CCC1=C(C=C(C=C1)C)C	C10H14	341.6	10.7	prediction	65.5
C10_Mono-Aromatics(6)		17877	2-ethyl-1,3-dimethylbenzene	CCC1=C(C=CC=C1C)C	C10H14	341.6	10.7	prediction	60.3
C10_Mono-Aromatics(7)		17877	2-ethyl-1,3-dimethylbenzene	CCC1=C(C=CC=C1C)C	C10H14	341.6	10.7	prediction	60.5
Benzene, 2,4-dimethyl-1-(1methylpropyl)-		15141	1-butan-2-yl-2,4-dimethylbenzene	CCC(C)C1=C(C=C(C=C1)C)C	C12H18	346.4	14.0	prediction	26.9
Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	1483-60-9	15141	1-butan-2-yl-2,4-dimethylbenzene	CCC(C)C1=C(C=C(C=C1)C)C	C12H18	346.4	14.0	prediction	26.9
1-t-Butyl-2-methylbenzene	1074-92-6	33712	1-tert-butyl-2-methylbenzene	CC1=CC=CC=C1C(C)(C)C	C11H16	352.5	17.3	prediction	60.0
Benzene, 1-(1,1-dimethylethyl)-3methyl-		33711	1-tert-butyl-3-methylbenzene	CC1=CC(=CC=C1)C(C)(C)C	C11H16	352.5	17.3	prediction	62.4
Benzene, 1-(1,1-dimethylethyl)-3-methyl-	1075-38-3	33711	1-tert-butyl-3-methylbenzene	CC1=CC(=CC=C1)C(C)(C)C	C11H16	352.5	17.3	prediction	62.4
C11_Mono-Aromatics(3)		33712	1-tert-butyl-2-methylbenzene	CC1=CC=CC=C1C(C)(C)C	C11H16	352.5	17.3	prediction	54.5
C11_Mono-Aromatics(4)		33712	1-tert-butyl-2-methylbenzene	CC1=CC=CC=C1C(C)(C)C	C11H16	352.5	17.3	prediction	54.5
C11_Mono-Aromatics(6)		33711	1-tert-butyl-3-methylbenzene	CC1=CC(=CC=C1)C(C)(C)C	C11H16	352.5	17.3	prediction	43.2
C11_Mono-Aromatics(7)		33711	1-tert-butyl-3-methylbenzene	CC1=CC(=CC=C1)C(C)(C)C	C11H16	352.5	17.3	prediction	62.4
1,3-diisopropylbenzene	99-62-7	7450	1,3-di(propan-2-yl)benzene	CC(C)C1=CC(=CC=C1)C(C)C	C12H18	353.3	14.0	experiment	43.0
Benzene, 1,4-dimethyl-2-(2methylpropyl)-		41508	1,4-dimethyl-2-(2-methylpropyl)benzene	CC1=CC(=C(C=C1)CC(C)C	C12H18	360.6	10.8	prediction	25.3
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	55669-88-0	41508	1,4-dimethyl-2-(2-methylpropyl)benzene	CC1=CC(=C(C=C1)CC(C)C	C12H18	360.6	10.8	prediction	25.3
C12_Mono-Aromatics(7)		41508	1,4-dimethyl-2-(2-methylpropyl)benzene	CC1=CC(=C(C=C1)CC(C)C	C12H18	360.6	10.8	prediction	41.8
C12_Mono-Aromatics(8)		41508	1,4-dimethyl-2-(2-methylpropyl)benzene	CC1=CC(=C(C=C1)CC(C)C	C12H18	360.6	10.8	prediction	41.8
1,3-diethyl-5-methyl benzene		16302	1,3-diethyl-5-methylbenzene	CCC1=CC(=CC(=C1)C)CC	C11H16	372.6	12.9	prediction	45.7
1,4-diethyl-2-methylbenzene	13632-94-5	139518	1,4-diethyl-2-methylbenzene	CCC1=CC(=C(C=C1)CC)C	C11H16	372.6	12.9	prediction	38.9
2,4-diethyl-1-methylbenzene	1758-85-6	0	2,4-diethyl-1-methylbenzene	CCC1=CC(=C(C=C1)C)CC	C11H16	372.6	12.9	prediction	39.8
Benzene, 1,3-diethyl-5-methyl-	2050-24-0	16302	1,3-diethyl-5-methylbenzene	CCC1=CC(=CC(=C1)C)CC	C11H16	372.6	12.9	prediction	43.2
C11_Mono-Aromatics(5)		16302	1,3-diethyl-5-methylbenzene	CCC1=CC(=CC(=C1)C)CC	C11H16	372.6	12.9	prediction	43.2
1,2-Diethylbenzene	135-01-3	8657	1,2-diethylbenzene	CCC1=CC=CC=C1CC	C10H14	376.3	14.7	experiment	71.5
C10_Mono-Aromatics(2)		8657	1,2-diethylbenzene	CCC1=CC=CC=C1CC	C10H14	376.3	14.7	experiment	71.5
C10_Mono-Aromatics(3)		8657	1,2-diethylbenzene	CCC1=CC=CC=C1CC	C10H14	376.3	14.7	experiment	71.5
1t-Butyl-4-ethylbenzene	7364-19-4	81828	1-tert-butyl-4-ethylbenzene	CCC1=CC=C(C=C1)C(C)(C)C	C12H18	383.4	18.0	prediction	34.2
C12_Mono-Aromatics(3)		81828	1-tert-butyl-4-ethylbenzene	CCC1=CC=C(C=C1)C(C)(C)C	C12H18	383.4	18.0	prediction	34.2
1,2,3,5-Tetramethylbenzene	527-53-7	10695	1,2,3,5-tetramethylbenzene	CC1=CC(=C(C(=C1)C)C)C	C10H14	386.2	14.8	experiment	47.5
1,2,4,5-Tetramethylbenzene	95-93-2	7269	1,2,4,5-tetramethylbenzene	CC1=CC(=C(C=C1C)C)C	C10H14	393.0	15.3	experiment	51.7
Benzene, 1,2,4-trimethyl-5-(1methylethyl)-			unknown	CC1=CC(=C(C=C1C)C(C)C)C	C12H18	401.2	15.1	prediction	27.8
C12_Mono-Aromatics(17)		0	unknown	CC1=CC(=C(C=C1C)C(C)C)C	C12H18	401.2	15.1	prediction	41.8
2-Methylindan	824-63-5	13213	2-methyl-2,3-dihydro-1H-indene	CC1CC2=CC=CC=C2C1	C10H12	402.4	18.6	prediction	53.8
1-ethyl-2,4,5-trimethylbenzen	17851-27-2	28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	27.4

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
1-Ethyl-2,4,5-Trimethylbenzene		28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	27.4
Benzene, 1-ethyl-2,4,5-trimethyl-		28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	32.8
C11_Mono-Aromatics(10)		28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	26.3
C11_Mono-Aromatics(11)		28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	26.3
C11_Mono-Aromatics(9)		28812	1-ethyl-2,4,5-trimethylbenzene	CCC1=C(C=C(C(=C1)C)C)C	C11H16	402.9	12.3	prediction	54.6
Ethyl-1,3,4-trimethyl benzene		528692	2-ethyl-1,3,4-trimethylbenzene	CCC1=C(C=CC(=C1C)C)C	C11H16	402.9	12.3	prediction	28.4
1,2,4-Triethylbenzene	877-44-1	13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	28.5
1,3,5-Triethylbenzene	102-25-0	7602	1,3,5-triethylbenzene	CCC1=CC(=CC(=C1)CC)CC	C12H18	403.5	16.4	prediction	31.9
C12_Mono-Aromatics(10)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	26.9
C12_Mono-Aromatics(11)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
C12_Mono-Aromatics(12)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
C12_Mono-Aromatics(13)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
C12_Mono-Aromatics(14)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
C12_Mono-Aromatics(15)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
C12_Mono-Aromatics(16)		13415	1,2,4-triethylbenzene	CCC1=CC(=C(C=C1)CC)CC	C12H18	403.5	16.4	prediction	41.8
2-Ethyl-2,3-dihydro-1H-indene	56147-63-8	41747	2-ethyl-2,3-dihydro-1H-indene	CCC1CC2=CC=CC=C2C1	C11H14	409.0	18.6	prediction	30.9
1,3,5-trimethyl-2-propylbenze	1062949	521228	1,3,5-trimethyl-2-propylbenzene	CCCC1=C(C=C(C=C1C)C)C	C12H18	409.5	12.3	prediction	19.3
1,3,5-Trimethyl-2-Propylbenze(1)	1062949	521228	1,3,5-trimethyl-2-propylbenzene	CCCC1=C(C=C(C=C1C)C)C	C12H18	409.5	12.3	prediction	19.3
1,3,5-trimethyl-2-propylbenzene	1062949	521228	1,3,5-trimethyl-2-propylbenzene	CCCC1=C(C=C(C=C1C)C)C	C12H18	409.5	12.3	prediction	19.3
methyl-tetralin		19755	2-methyl-1,2,3,4-tetrahydronaphthalene	CC1CCC2=CC=CC=C2C1	C11H14	409.7	18.6	prediction	22.0
Naphthalene, 1,2,3,4-tetrahydr	3877-19-8	19755	2-methyl-1,2,3,4-tetrahydronaphthalene	CC1CCC2=CC=CC=C2C1	C11H14	409.7	18.6	prediction	26.6
Naphthalene, 1,2,3,4-tetrahydro-2methyl-		19755	2-methyl-1,2,3,4-tetrahydronaphthalene	CC1CCC2=CC=CC=C2C1	C11H14	409.7	18.6	prediction	26.3
1-Methyl-4-t-butylbenzene	98-51-1	7390	1-tert-butyl-4-methylbenzene	CC1=CC=C(C=C1)C(C)(C)C	C11H16	410.8	15.9	experiment	56.2
1-methyl-4-tert-butylbenzene	98-51-1	7390	1-tert-butyl-4-methylbenzene	CC1=CC=C(C=C1)C(C)(C)C	C11H16	410.8	15.9	experiment	56.2
1-t-Butyl-3,5-dimethylbenzene	98-19-1	7378	1-tert-butyl-3,5-dimethylbenzene	CC1=CC(=CC(=C1)C(C)(C)C)C	C12H18	413.8	17.9	prediction	37.7
C12_Mono-Aromatics(2)		7378	1-tert-butyl-3,5-dimethylbenzene	CC1=CC(=CC(=C1)C(C)(C)C)C	C12H18	413.8	17.9	prediction	37.7
C12_Indanes(8)		36111	2-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1CCC2=CC=CC=C2C1	C12H16	416.3	18.6	prediction	16.9
Naphthalene, 2-ethyl-1,2,3,4tetrahydro-		36111	2-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1CCC2=CC=CC=C2C1	C12H16	416.3	18.6	prediction	17.7
Benzene, 1-(1-methylethenyl)-2-(1methylethyl)-		589341	1-propan-2-yl-2-prop-1-en-2-ylbenzene	CC(C)C1=CC=CC=C1C(=C)C	C12H16	417.6	27.4	prediction	21.3
Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	5557-93-7	589341	1-propan-2-yl-2-prop-1-en-2-ylbenzene	CC(C)C1=CC=CC=C1C(=C)C	C12H16	417.6	27.4	prediction	21.3
Benzene, 1-(1-methylethenyl)-4-(1methylethyl)-		16952	1-propan-2-yl-4-prop-1-en-2-ylbenzene	CC(C)C1=CC=C(C=C1)C(=C)C	C12H16	417.6	27.4	prediction	26.9
Benzene, 1-(1-methylethenyl)-4-(1-methylethyl)-	2388-14-9	16952	1-propan-2-yl-4-prop-1-en-2-ylbenzene	CC(C)C1=CC=C(C=C1)C(=C)C	C12H16	417.6	27.4	prediction	26.9
Benzene, 4-ethenyl-1,2-dimethyl-		33937	4-ethenyl-1,2-dimethylbenzene	CC1=C(C=C(C=C1)C=C)C	C10H12	419.8	13.6	prediction	47.8
1H-Indene,2,3-dihydro-2,2-dime	20836-11-7	140767	2,2-dimethyl-1,3-dihydroindene	CC1(CC2=CC=CC=C2C1)C	C11H14	420.8	19.9	prediction	45.2
C14_Mono-Aromatics(1)		90961365	1,2,5-trimethyl-3-pentylbenzene	CCCCCC1=CC(=CC(=C1C)C)C	C14H22	422.7	12.3	prediction	4.3
C14_Mono-Aromatics(2)		90961365	1,2,5-trimethyl-3-pentylbenzene	CCCCCC1=CC(=CC(=C1C)C)C	C14H22	422.7	12.3	prediction	9.0
C14_Mono-Aromatics(3)		90961365	1,2,5-trimethyl-3-pentylbenzene	CCCCCC1=CC(=CC(=C1C)C)C	C14H22	422.7	12.3	prediction	3.9
1,1-Dimethyl Indane	4912-92-9	78624	3,3-dimethyl-1,2-dihydroindene	CC1(CCC2=CC=CC=C21)C	C11H14	428.1	17.2	outlier	18.3
1H-Indene, 1-ethyl-2,3-dihydro-1methyl-		41840	3-ethyl-3-methyl-1,2-dihydroindene	CCC1(CCC2=CC=CC=C21)C	C12H16	434.7	17.2	outlier	30.0
Naphthalene, 1,2,3,4-tetrahydro-1,1dimethyl-		16137	4,4-dimethyl-2,3-dihydro-1H-naphthalene	CC1(CCCC2=CC=CC=C21)C	C12H16	435.5	17.2	outlier	26.0
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	1985-59-7	16137	4,4-dimethyl-2,3-dihydro-1H-naphthalene	CC1(CCCC2=CC=CC=C21)C	C12H16	435.5	17.2	outlier	26.0
(2-methyl-1-propenyl)-benzene	768-49-0	13030	2-methylprop-1-enylbenzene	CC(=CC1=CC=CC=C1)C	C10H12	436.9	16.6	experiment	63.8
Benzene, (2-methyl-1-propenyl)-		13030	2-methylprop-1-enylbenzene	CC(=CC1=CC=CC=C1)C	C10H12	436.9	16.6	experiment	63.8
2,3-Dihydroindene		10326	2,3-dihydro-1H-indene	C1CC2=CC=CC=C2C1	C9H10	439.5	16.6	experiment	96.3
Indan	496-11-7	10326	2,3-dihydro-1H-indene	C1CC2=CC=CC=C2C1	C9H10	439.5	16.6	experiment	85.4
indane	496-11-7	10326	2,3-dihydro-1H-indene	C1CC2=CC=CC=C2C1	C9H10	439.5	16.6	experiment	85.4
4-Methylindan	824-22-6	13211	4-methyl-2,3-dihydro-1H-indene	CC1=C2CCCC2=CC=C1	C10H12	450.5	18.6	prediction	39.6
5-Methylindan	874-35-1	13402	5-methyl-2,3-dihydro-1H-indene	CC1=CC2=C(CCC2)C=C1	C10H12	450.5	18.6	prediction	42.4
Benzene, 3-ethyl-1,2,4,5-tetramethyl-		590293	3-ethyl-1,2,4,5-tetramethylbenzene	CCC1=C(C(=CC(=C1C)C)C)C	C12H18	464.2	14.4	prediction	12.3
Naphthalene	91-20-3	931	naphthalene	C1=CC=C2C=CC=CC2=C1	C10H8	466.1	8.4	experiment	26.0
1-H-Indene		7219	1H-indene	C1C=CC2=CC=CC=C21	C9H8	467.7	17.8	experiment	247.4
Indene	95-13-6	7219	1H-indene	C1C=CC2=CC=CC=C21	C9H8	467.7	17.8	experiment	75.0
C12_Indanes(7)		522578	2,6-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1CCC2=C(C1)C=CC(=C2)C	C12H16	471.0	18.7	prediction	17.0

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
Naphthalene, 1,2,3,4-tetrahydro-2,6dimethyl-		522578	2,6-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1CCC2=C(C1)C=CC(=C2)C	C12H16	471.0	18.7	prediction	12.0
1H-Indene, 1-methyl-	767-59-9	13024	1-methyl-1H-indene	CC1C=CC2=CC=CC=C12	C10H10	479.1	32.9	outlier	56.5
1H-Indene, 3-methyl-	767-59-9	13024	1-methyl-1H-indene	CC1C=CC2=CC=CC=C12	C10H10	479.1	32.9	outlier	40.1
C10_Indenes(1)		13024	1-methyl-1H-indene	CC1C=CC2=CC=CC=C12	C10H10	479.1	32.9	outlier	56.5
α,ß,ß-Trimethylstyrene		13036	2-ethenyl-1,3,5-trimethylbenzene	CC1=CC(=C(C(=C1)C)C=C)C	C11H14	481.1	14.9	prediction	57.9
Pentamethylbenzene	700-12-9	12784	1,2,3,4,5-pentamethylbenzene	CC1=CC(=C(C(=C1C)C)C)C	C11H16	481.8	18.4	experiment	21.0
1-H-Indene-1-Ethyl	6953-66-8	236404	1-ethyl-1H-indene	CCC1C=CC2=CC=CC=C12	C11H12	485.6	32.9	outlier	18.6
Diimethyl Indene - 2		236404	1-ethyl-1H-indene	CCC1C=CC2=CC=CC=C12	C11H12	485.6	32.9	outlier	20.4
Dimethyl Indene - 1		236404	1-ethyl-1H-indene	CCC1C=CC2=CC=CC=C12	C11H12	485.6	32.9	outlier	32.7
Dimethyl Indene - 2		236404	1-ethyl-1H-indene	CCC1C=CC2=CC=CC=C12	C11H12	485.6	32.9	outlier	31.9
Dimethyl Indene - 3		236404	1-ethyl-1H-indene	CCC1C=CC2=CC=CC=C12	C11H12	485.6	32.9	outlier	31.5
1H-Indene, 2,3-dihydro-4-propyl-	92013-16-6	583029	4-propyl-2,3-dihydro-1H-indene	CCCC1=CC=CC2=C1CCC2	C12H16	488.0	19.1	prediction	11.8
n-propyl indane		13330218	5-propyl-2,3-dihydro-1H-indene	CCCC1=CC2=C(CCC2)C=C1	C12H16	488.0	19.1	prediction	18.3
5-Ethyltetralin		54756	5-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC=CC2=C1CCCC2	C12H16	488.8	19.1	prediction	10.4
6-ethyl-1,2,3,4-tetrahydronap		31189	6-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC2=C(CCCC2)C=C1	C12H16	488.8	19.1	prediction	12.3
6-ethylTetralin		31189	6-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC2=C(CCCC2)C=C1	C12H16	488.8	19.1	prediction	14.8
Naphthalene, 5-ethyl-1,2,3,4-t	42775-75-7	54756	5-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC=CC2=C1CCCC2	C12H16	488.8	19.1	prediction	15.2
Naphthalene, 5-ethyl-1,2,3,4tetrahydro-		54756	5-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC=CC2=C1CCCC2	C12H16	488.8	19.1	prediction	15.2
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	42775-75-7	54756	5-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC=CC2=C1CCCC2	C12H16	488.8	19.1	prediction	15.2
Naphthalene, 6-ethyl-1,2,3,4tetrahydro-		31189	6-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1=CC2=C(CCCC2)C=C1	C12H16	488.8	19.1	prediction	12.6
1H-Indene, 2,3-dihydro-1,1,4-trimethyl-	16204-72-1	589442	3,3,7-trimethyl-1,2-dihydroindene	CC1=C2CCC(C2=CC=C1)(C)C	C12H16	489.4	17.6	outlier	13.5
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	40650-41-7	589447	3,3,6-trimethyl-1,2-dihydroindene	CC1=CC2=C(C=C1)C(CC2)(C)C	C12H16	489.4	17.6	outlier	12.8
1H-Indene, 2,3-dihydro-1,1,6-trimethyl-		589441	3,3,5-trimethyl-1,2-dihydroindene	CC1=CC2=C(CCC2(C)C)C=C1	C12H16	489.4	17.6	outlier	13.5
C12_Indanes(2)		589442	3,3,7-trimethyl-1,2-dihydroindene	CC1=C2CCC(C2=CC=C1)(C)C	C12H16	489.4	17.6	outlier	13.7
C12_Indanes(3)		589442	3,3,7-trimethyl-1,2-dihydroindene	CC1=C2CCC(C2=CC=C1)(C)C	C12H16	489.4	17.6	outlier	12.8
C12_Indanes(4)		589442	3,3,7-trimethyl-1,2-dihydroindene	CC1=C2CCC(C2=CC=C1)(C)C	C12H16	489.4	17.6	outlier	12.8
1-Methylindan		13023	1-methyl-2,3-dihydro-1H-indene	CC1CCC2=CC=CC=C12	C10H12	492.4	26.3	prediction	67.9
C10_Indanes(1)		13023	1-methyl-2,3-dihydro-1H-indene	CC1CCC2=CC=CC=C12	C10H12	492.4	26.3	prediction	89.0
C1-Indane - 1		13023	1-methyl-2,3-dihydro-1H-indene	CC1CCC2=CC=CC=C12	C10H12	492.4	26.3	prediction	2.7
Indan, 1-methyl-	767-58-8	13023	1-methyl-2,3-dihydro-1H-indene	CC1CCC2=CC=CC=C12	C10H12	492.4	26.3	prediction	55.3
C13_Indanes(1)		297000	6-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1=CC2=C(CCCC2)C=C1	C13H18	495.3	19.1	prediction	12.7
C3-tetralin		297000	6-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1=CC2=C(CCCC2)C=C1	C13H18	495.3	19.1	prediction	15.3
C3-Tetralin-2		297000	6-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1=CC2=C(CCCC2)C=C1	C13H18	495.3	19.1	prediction	49.9
Naphthalene, 1,2,3,4-tetrahydro-6propyl-		297000	6-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1=CC2=C(CCCC2)C=C1	C13H18	495.3	19.1	prediction	7.3
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	42775-77-9	297000	6-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1=CC2=C(CCCC2)C=C1	C13H18	495.3	19.1	prediction	7.3
1H-Indene, 1-ethyl-2,3-dihydro-	4830-99-3	20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	25.6
5-Ethyl Indane		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	23.9
C11_Indanes(1)		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	21.1
C11_Indanes(2)		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	36.9
C2 Indane - 1		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	23.8
Dimethyl Indane - 1		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	30.9
Dimethyl Indane - 2		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	29.9
Dimethyl Indane - 3		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	19.5
Dimethyl Indane - 4		20971	1-ethyl-2,3-dihydro-1H-indene	CCC1CCC2=CC=CC=C12	C11H14	499.0	26.3	prediction	19.1
Naphthalene, 1,2,3,4-tetrahydro-1methyl-		15262	1-methyl-1,2,3,4-tetrahydronaphthalene	CC1CCCC2=CC=CC=C12	C11H14	499.7	26.3	prediction	26.7
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	1559-81-5	15262	1-methyl-1,2,3,4-tetrahydronaphthalene	CC1CCCC2=CC=CC=C12	C11H14	499.7	26.3	prediction	26.7
1H-Indene, 2,3-dihydro-1,2-dim		28225	1,2-dimethyl-2,3-dihydro-1H-indene	CC1CC2=CC=CC=C2C1C	C11H14	505.6	26.6	prediction	39.9
1H-Indene, 2,3-dihydro-1,2-dimethyl		28225	1,2-dimethyl-2,3-dihydro-1H-indene	CC1CC2=CC=CC=C2C1C	C11H14	505.6	26.6	prediction	39.9
Naphthalene, 1-ethyl-1,2,3,4tetrahydro-		139497	1-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1CCCC2=CC=CC=C12	C12H16	506.3	26.3	prediction	15.5
Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-	13556-58-6	139497	1-ethyl-1,2,3,4-tetrahydronaphthalene	CCC1CCCC2=CC=CC=C12	C12H16	506.3	26.3	prediction	15.5
1H-Indene, 2,3-dihydro-4,6-dimethyl-	1685-82-1	15518	4,6-dimethyl-2,3-dihydro-1H-indene	CC1=CC(=C2CCCC2=C1)C	C11H14	511.8	19.2	prediction	23.5
1H-Indene, 2,3-dihydro-5,6-dimethyl-	1075-22-5	70635	5,6-dimethyl-2,3-dihydro-1H-indene	CC1=CC2=C(CCC2)C=C1C	C11H14	511.8	19.2	prediction	21.9
4,7-Dimethyl Indan		23151	4,7-dimethyl-2,3-dihydro-1H-indene	CC1=C2CCCC2=C(C=C1)C	C11H14	511.8	19.2	prediction	21.7

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
4,7-Dimethyl Indane	6682-71-9	23151	4,7-dimethyl-2,3-dihydro-1H-indene	CC1=C2CCCC2=C(C=C1)C	C11H14	511.8	19.2	prediction	22.5
4,7-DimethylIndane		23151	4,7-dimethyl-2,3-dihydro-1H-indene	CC1=C2CCCC2=C(C=C1)C	C11H14	511.8	19.2	prediction	21.7
propyl tetralin		582936	1-propyl-1,2,3,4-tetrahydronaphthalene	CCCC1CCCC2=CC=CC=C12	C13H18	512.9	26.3	prediction	9.6
Naphthalene, 1,2,3,4-tetrahydro-5,6dimethyl-		589445	5,6-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1=C(C2=C(CCCC2)C=C1)C	C12H16	519.1	19.2	prediction	9.9
Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-	20027-77-4	589445	5,6-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1=C(C2=C(CCCC2)C=C1)C	C12H16	519.1	19.2	prediction	9.9
1,1,3-Trimethyl Indan		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	17.8
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	2613-76-5	17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	34.0
C12_Indanes(1)		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	18.3
C12_Indanes(9)		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	82.4
C2-Tetralin-1		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	10.6
C2-Tetralin-2		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	10.6
C3 Indane - 6		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	9.0
C3-Indane-2		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	21.7
Trimethyl Indane - 4		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	16.9
Trimethyl Indene - 2		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	21.5
Trimethyl Indene - 3		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	22.8
Trimethyl Indene - 4		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	21.6
Trimethyl Indene - 5		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	19.6
Trimethyl Indene - 6		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	19.2
Trimethyl Indene - 7		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	18.1
Trimethyl Indene - 8		17470	1,3,3-trimethyl-1,2-dihydroindene	CC1CC(C2=CC=CC=C12)(C)C	C12H16	531.3	29.5	outlier	16.6
1,6-Dimethyl Indan		28231	1,6-dimethyl-2,3-dihydro-1H-indene	CC1CCC2=C1C=C(C=C2)C	C11H14	553.7	26.5	prediction	25.6
1H-Indene, 2,3-dihydro-1,6-dimethyl-		28231	1,6-dimethyl-2,3-dihydro-1H-indene	CC1CCC2=C1C=C(C=C2)C	C11H14	553.7	26.5	prediction	32.4
Naphthalene, 1,2,3,4-tetrahydro-1,8dimethyl-		32970	1,8-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1CCCC2=CC=CC(=C12)C	C12H16	561.0	26.5	prediction	14.6
C12_Indanes(5)		23150	4,5,7-trimethyl-2,3-dihydro-1H-indene	CC1=CC(=C2CCCC2=C1C)C	C12H16	573.1	20.1	prediction	19.2
C12_Indanes(6)		23150	4,5,7-trimethyl-2,3-dihydro-1H-indene	CC1=CC(=C2CCCC2=C1C)C	C12H16	573.1	20.1	prediction	19.2
Indane,4,5,7-trimethyl	6682-06-0	23150	4,5,7-trimethyl-2,3-dihydro-1H-indene	CC1=CC(=C2CCCC2=C1C)C	C12H16	573.1	20.1	prediction	11.8
1-H-Indene,1-3-dimethyl	2177-48-2	582329	1,3-dimethyl-1H-indene	CC1C=C(C2=CC=CC=C12)C	C11H12	591.2	30.4	outlier	21.1
1H-Indene, 2,3-dihydro-1,3-dimethyl-	4175-53-5	20143	1,3-dimethyl-2,3-dihydro-1H-indene	CC1CC(C2=CC=CC=C12)C	C11H14	595.6	49.8	prediction	36.9
1,4-dimethyl-1,2,3,4-tetrahyd		138145	1,4-dimethyl-1,2,3,4-tetrahydronaphthalene	CC1CCC(C2=CC=CC=C12)C	C12H16	602.9	49.7	prediction	12.4
1,1’-Biphenyl		7095	1,1'-biphenyl	C1=CC=C(C=C1)C2=CC=CC=C2	C12H10	612.5	22.9	experiment	9.8
1,1'-Biphenyl		7095	1,1'-biphenyl	C1=CC=C(C=C1)C2=CC=CC=C2	C12H10	612.5	22.9	experiment	9.8
biphenyl	92-52-4	7095	1,1'-biphenyl	C1=CC=C(C=C1)C2=CC=CC=C2	C12H10	612.5	22.9	experiment	9.8
1H-Indene, 2,3-dihydro-1,4,7-trimethyl-	54340-87-3	41052	1,4,7-trimethyl-2,3-dihydro-1H-indene	CC1CCC2=C(C=CC(=C12)C)C	C12H16	615.0	27.0	prediction	17.0
1H-Indene, 2,3-dihydro-1,5,7-trimethyl-		37476	1,5,7-trimethyl-2,3-dihydro-1H-indene	CC1CCC2=CC(=CC(=C12)C)C	C12H16	615.0	27.0	prediction	16.7
1-Methylnaphthalene	90-12-0	7002	1-methylnaphthalene	CC1=CC=CC2=CC=CC=C12	C11H10	649.1	24.7	experiment	15.4
2-Methylnaphthalene	91-57-6	7055	2-methylnaphthalene	CC1=CC2=CC=CC=C2C=C1	C11H10	649.1	24.7	experiment	15.3
C13_Naphthalenes(5)		16238	2-propan-2-ylnaphthalene	CC(C)C1=CC2=CC=CC=C2C=C1	C13H14	649.5	16.1	prediction	6.8
Naphthalene, 2-(1-methylethyl)-	2027-17-0	16238	2-propan-2-ylnaphthalene	CC(C)C1=CC2=CC=CC=C2C=C1	C13H14	649.5	16.1	prediction	6.8
Naphthalene, 1-propyl-	2765-18-6	33800	1-propylnaphthalene	CCCC1=CC=CC2=CC=CC=C21	C13H14	657.8	12.9	prediction	5.2
Benzene, 1-methyl-4-(phenylmethyl)-	620-83-7	69290	1-benzyl-4-methylbenzene	CC1=CC=C(C=C1)CC2=CC=CC=C2	C14H14	669.7	33.4	prediction	4.0
1,8-dimethyl-1,2,3,4-tetrahydronaphthalene	569-41-5	11287	1,8-dimethylnaphthalene	CC1=C2C(=CC=CC2=CC=C1)C	C12H12	681.6	12.7	prediction	6.1
Naphthalene, 1,6-dimethyl-	575-43-9	11328	1,6-dimethylnaphthalene	CC1=CC2=CC=CC(=C2C=C1)C	C12H12	681.6	12.7	prediction	7.3
Naphthalene, 1,7-dimethyl-		11326	1,7-dimethylnaphthalene	CC1=CC2=C(C=CC=C2C=C1)C	C12H12	681.6	12.7	prediction	7.7
Naphthalene, 1,8-dimethyl-	569-41-5	11287	1,8-dimethylnaphthalene	CC1=C2C(=CC=CC2=CC=C1)C	C12H12	681.6	12.7	prediction	6.1
Naphthalene,1,7-dimethyl	575-37-1	11326	1,7-dimethylnaphthalene	CC1=CC2=C(C=CC=C2C=C1)C	C12H12	681.6	12.7	prediction	7.8
Naphthalene,2,7 dimethyl	582-16-1	11396	2,7-dimethylnaphthalene	CC1=CC2=C(C=C1)C=CC(=C2)C	C12H12	681.6	12.7	prediction	7.7
2-Ethylnaphthalene	939-27-5	13652	2-ethylnaphthalene	CCC1=CC2=CC=CC=C2C=C1	C12H12	701.3	26.6	experiment	9.0
1,4-dimethylnaphthalene	571-58-4	11304	1,4-dimethylnaphthalene	CC1=CC=C(C2=CC=CC=C12)C	C12H12	711.8	26.7	experiment	6.5
Naphthalene-1,4-dimethyl		11304	1,4-dimethylnaphthalene	CC1=CC=C(C2=CC=CC=C12)C	C12H12	711.8	26.7	experiment	7.7
Naphthalene, 2-ethenyl-	827-54-3	13230	2-ethenylnaphthalene	C=CC1=CC2=CC=CC=C2C=C1	C12H10	729.4	15.7	prediction	6.2
Benzene, 1-methyl-3-[(4methylphenyl)methyl]-		602495	1-methyl-3-[(4-methylphenyl)methyl]benzene	CC1=CC=C(C=C1)CC2=CC=CC(=C2)C	C15H16	731.0	33.7	prediction	3.2
1-Ethylnaphthalene	1127-76-0	14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	8.7

Compound Name (as it appears in DHA)	CAS NO	CID	IUPAC Name	Canonical SMILES	Molecular Formula	YSI	YSI Error	Prediction Type	VP_{443K} (kPa)
Dimethylnaphthalene - 6		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	7.5
Dimethylnaphthalene-3		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	8.7
Dimethylnaphthalene-4		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	8.4
Dimethylnaphthalene-5		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	7.7
Dimethylnaphthalene-5(1)		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	7.7
Dimethylnaphthalene-6		14315	1-ethylnaphthalene	CCC1=CC=CC2=CC=CC=C21	C12H12	732.7	27.4	experiment	6.2
C13_Naphthalenes(3)		16479	1,4,6-trimethylnaphthalene	CC1=CC2=C(C=CC(=C2C=C1)C)C	C13H14	742.9	13.6	prediction	4.3
C13_Naphthalenes(4)		16478	1,4,5-trimethylnaphthalene	CC1=C2C(=CC=C(C2=CC=C1)C)C	C13H14	742.9	13.6	prediction	3.6
Naphthalene, 1,4,5-trimethyl-	2131-41-1	16478	1,4,5-trimethylnaphthalene	CC1=C2C(=CC=C(C2=CC=C1)C)C	C13H14	742.9	13.6	prediction	3.2
Naphthalene, 1,4,6-trimethyl-	2131-42-2	16479	1,4,6-trimethylnaphthalene	CC1=CC2=C(C=CC(=C2C=C1)C)C	C13H14	742.9	13.6	prediction	4.3
Naphthalene, 1,6,7-trimethyl-	2245-38-7	16732	1,6,7-trimethylnaphthalene	CC1=C2C=C(C(=CC2=CC=C1)C)C	C13H14	742.9	13.6	prediction	3.6
Naphthalene, 2,3,6-trimethyl-	829-26-5	13237	2,3,6-trimethylnaphthalene	CC1=CC2=C(C=C1)C=C(C(=C2)C)C	C13H14	742.9	13.6	prediction	7.6
1,2-dimethylnaphthalene	573-98-8	11317	1,2-dimethylnaphthalene	CC1=C(C2=CC=CC=C2C=C1)C	C12H12	743.1	28.0	experiment	6.6
1,3-dimethylnaphthalene	575-41-7	11327	1,3-dimethylnaphthalene	CC1=CC2=CC=CC=C2C(=C1)C	C12H12	743.1	28.0	experiment	7.7
Naphthalene, 1,2-dimethyl-		11317	1,2-dimethylnaphthalene	CC1=C(C2=CC=CC=C2C=C1)C	C12H12	743.1	28.0	experiment	6.9
Naphthalene, 1,3-dimethyl-		11327	1,3-dimethylnaphthalene	CC1=CC2=CC=CC=C2C(=C1)C	C12H12	743.1	28.0	experiment	7.7
C14_Naphthalenes(1)		3017163	2,6-diethylnaphthalene	CCC1=CC2=C(C=C1)C=C(C=C2)CC	C14H16	743.5	15.5	prediction	4.0
Naphthalene, 2,6-diethyl	59919-41-4	3017163	2,6-diethylnaphthalene	CCC1=CC2=C(C=C1)C=C(C=C2)CC	C14H16	743.5	15.5	prediction	2.7
2,3-dimethylnaphthalene	581-40-8	11386	2,3-dimethylnaphthalene	CC1=CC2=CC=CC=C2C=C1C	C12H12	748.4	28.0	experiment	6.4
Naphthalene, 2,3-dimethyl-		11386	2,3-dimethylnaphthalene	CC1=CC2=CC=CC=C2C=C1C	C12H12	748.4	28.0	experiment	6.8
1,1’-Biphenyl, 4-methyl-		12566	1-methyl-4-phenylbenzene	CC1=CC=C(C=C1)C2=CC=CC=C2	C13H12	769.3	28.7	experiment	6.6
4-methylbiphenyl	644-08-6	12566	1-methyl-4-phenylbenzene	CC1=CC=C(C=C1)C2=CC=CC=C2	C13H12	769.3	28.7	experiment	6.6
2,6-dimethylnaphthalene	581-42-0	11387	2,6-dimethylnaphthalene	CC1=CC2=C(C=C1)C=C(C=C2)C	C12H12	774.5	29.2	experiment	7.9
Naphthalene,2,6 dimethyl		11387	2,6-dimethylnaphthalene	CC1=CC2=C(C=C1)C=C(C=C2)C	C12H12	774.5	29.2	experiment	7.9
1,5-dimethylnaphthalene	571-61-9	11306	1,5-dimethylnaphthalene	CC1=C2C=CC=C(C2=CC=C1)C	C12H12	779.7	29.3	experiment	7.1
Naphthalene, 1,5-dimethyl-		11306	1,5-dimethylnaphthalene	CC1=C2C=CC=C(C2=CC=C1)C	C12H12	779.7	29.3	experiment	7.1
1,1’-Biphenyl, 3-methyl-		12564	1-methyl-3-phenylbenzene	CC1=CC(=CC=C1)C2=CC=CC=C2	C13H12	779.7	29.3	experiment	5.7
3-methylbiphenyl	643-93-6	12564	1-methyl-3-phenylbenzene	CC1=CC(=CC=C1)C2=CC=CC=C2	C13H12	779.7	29.3	experiment	5.7
1,4,6,7-tetramethylnaphthalene		3014782	1,4,6,7-tetramethylnaphthalene	CC1=C2C=C(C(=CC2=C(C=C1)C)C)C	C14H16	804.2	15.0	prediction	2.1
acenaphthene	83-32-9	6734	1,2-dihydroacenaphthylene	C1CC2=CC=CC3=C2C1=CC=C3	C12H10	805.8	30.5	experiment	19.8
1,1’-Biphenyl, 2,4’-dimethyl-		123078	1-methyl-2-(4-methylphenyl)benzene	CC1=CC=C(C=C1)C2=CC=CC=C2C	C14H14	810.4	14.0	prediction	4.3
1,1’-Biphenyl, 3,4’-dimethyl-		20492	1,2-dimethyl-4-phenylbenzene	CC1=C(C=C(C=C1)C2=CC=CC=C2)C	C14H14	810.4	14.0	prediction	3.9
1,1'-Biphenyl, 2,3'-dimethyl-	611-43-8	69142	1-methyl-2-(3-methylphenyl)benzene	CC1=CC(=CC=C1)C2=CC=CC=C2C	C14H14	810.4	14.0	prediction	5.6
1,1'-Biphenyl, 2,4'-dimethyl-	611-61-0	123078	1-methyl-2-(4-methylphenyl)benzene	CC1=CC=C(C=C1)C2=CC=CC=C2C	C14H14	810.4	14.0	prediction	4.3
1,1'-Biphenyl, 3,4'-dimethyl-	7383-90-6	23859	1-methyl-3-(4-methylphenyl)benzene	CC1=CC=C(C=C1)C2=CC=CC(=C2)C	C14H14	810.4	14.0	prediction	3.9
4-Ethylbiphenyl	5707-44-8	79786	1-ethyl-4-phenylbenzene	CCC1=CC=C(C=C1)C2=CC=CC=C2	C14H14	811.1	30.5	experiment	3.1
Azulene, 4,6,8-trimethyl-	941-81-1	70333	4,6,8-trimethylazulene	CC1=CC(=C2C=CC=C2C(=C1)C)C	C13H14	829.4	15.3	prediction	3.8
C13_Naphthalenes(1)		70333	4,6,8-trimethylazulene	CC1=CC(=C2C=CC=C2C(=C1)C)C	C13H14	829.4	15.3	prediction	6.8
C13_Naphthalenes(2)		70333	4,6,8-trimethylazulene	CC1=CC(=C2C=CC=C2C(=C1)C)C	C13H14	829.4	15.3	prediction	6.8
C13_Naphthalenes(6)		70333	4,6,8-trimethylazulene	CC1=CC(=C2C=CC=C2C(=C1)C)C	C13H14	829.4	15.3	prediction	3.6
C13_Naphthalenes(7)		70333	4,6,8-trimethylazulene	CC1=CC(=C2C=CC=C2C(=C1)C)C	C13H14	829.4	15.3	prediction	3.6
1,1’-Biphenyl, 2-methyl-		12563	1-methyl-2-phenylbenzene	CC1=CC=CC=C1C2=CC=CC=C2	C13H12	863.3	32.5	experiment	9.7
4,4’-Dimethylbiphenyl		11941	1-methyl-4-(4-methylphenyl)benzene	CC1=CC=C(C=C1)C2=CC=C(C=C2)C	C14H14	899.9	51.2	experiment	2.7
3,3’-Dimethylbiphenyl	612-75-9	11931	1-methyl-3-(3-methylphenyl)benzene	CC1=CC(=CC=C1)C2=CC=CC(=C2)C	C14H14	931.3	52.9	experiment	3.7
2,2’-Dimethylbiphenyl	605-39-0	11797	1-methyl-2-(2-methylphenyl)benzene	CC1=CC=CC=C1C2=CC=CC=C2C	C14H14	983.5	36.9	experiment	9.0

APPENDIX C

NEW PME VALUES FOR THE EXPERIMENTAL FUELS

Table C-1
$PME_{99.9}$ Values for Experimental Fuels in CRC Emission Studies

		Based on SwRI/Other DHA			Based on SSI DHA		
Program	**Fuel**	**Honda PMI**	**PME SIDI**	**PME PFI**	**Honda PMI**	**PME SIDI**	**PME PFI**
E94-2	A	1.41	1.63	1.16	1.44	1.58	1.17
	B	2.59	2.38	1.90	3.00	2.25	1.89
	E	1.40	1.62	1.04	1.35	1.47	1.01
	F	2.55	2.16	1.63	2.96	2.13	1.67
	C	1.29	1.74	1.21	1.24	1.60	1.15
	D	2.50	2.26	1.80	2.81	2.18	1.80
	G	1.26	1.58	1.03	1.23	1.53	1.02
	H	2.43	2.09	1.56	2.79	2.11	1.64
RW-107-3 SWRI Dataset	Fuel A	1.71	1.68	1.29	1.87	1.68	1.32
	Fuel B	1.10	1.41	0.98	1.19	1.43	1.02
	Fuel C	1.89	2.03	1.52	1.90	1.92	1.47
	Fuel D	0.67	0.98	0.64	0.67	0.98	0.64
	Fuel E	1.76	1.86	1.43	1.73	1.83	1.41
	Fuel F	1.07	1.48	1.03	1.07	1.45	1.03
	Fuel G	1.78	2.03	1.53	1.82	1.95	1.49
	Fuel H	0.64	1.07	0.69	0.66	1.10	0.72
	Fuel I	1.62	1.93	1.45	1.68	2.01	1.51
	Fuel J	2.49	2.26	1.64	2.56	2.14	1.59
	Fuel K	0.87	1.18	0.74	0.85	1.18	0.74
	Fuel L	2.25	2.17	1.70	2.35	2.16	1.71

Table C-2
$PME_{99.9}$ Values for Experimental Fuels in the EPAct Emission Study
(Strikeout Indicates Fuels Not Included in New PME Analysis)

Program	Fuel	Honda PMI	PME PFI	PME SIDI
EPAct	Fuel 1	0.67	0.92	0.60
	~~Fuel 2~~	~~1.04~~	~~1.43~~	~~0.76~~
	Fuel 3	0.72	1.04	0.68
	~~Fuel 4~~	~~0.95~~	~~1.30~~	~~0.81~~
	Fuel 5	1.16	1.69	0.99
	~~Fuel 6~~	~~0.93~~	~~1.29~~	~~0.77~~
	Fuel 7	0.80	1.07	0.64
	~~Fuel 8~~	~~0.80~~	~~1.10~~	~~0.61~~
	Fuel 9	1.46	1.72	1.11
	~~Fuel 10~~	~~1.47~~	~~2.10~~	~~1.41~~
	Fuel 11	1.01	1.45	0.97
	Fuel 12	1.46	1.73	1.27
	Fuel 13	1.51	1.96	1.24
	~~Fuel 14~~	~~1.00~~	~~1.26~~	~~0.72~~
	Fuel 15	0.98	1.32	0.81
	Fuel 16	0.98	1.45	0.96
	Fuel 20	0.59	1.01	0.64
	Fuel 21	0.89	1.54	0.98
	Fuel 22	0.57	0.97	0.61
	~~Fuel 23~~	~~0.82~~	~~1.28~~	~~0.76~~
	~~Fuel 24~~	~~0.75~~	~~1.15~~	~~0.67~~
	Fuel 25	1.18	1.83	1.23
	Fuel 26	1.30	1.69	1.21
	~~Fuel 27~~	~~0.84~~	~~1.24~~	~~0.74~~
	Fuel 28	0.94	1.49	0.98
	Fuel 30	1.12	1.47	1.03
	Fuel 31	1.07	1.73	1.15