

CRC Report No. RW-107-3a

**VALIDATION OF THE NEW PM
INDEX
FORMULA: PHASE 2**

Final Report

September 2023



**COORDINATING RESEARCH COUNCIL, INC.
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CRC Project No. RW-107-3a:

**VALIDATION OF THE NEW PM INDEX
FORMULA: PHASE 2**

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September 2023

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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 I¹ 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

| $\text{LA92 Phase 1 PM} = A_{\text{Veh}} \cdot \text{PME}_{\text{Eng Tech}} \quad \text{1.0} \quad \text{Direct Proportionality}$ | | | | | | | |
|--|----------|-------------------|-----------------|------------------|---------------------|---------------------|-------|
| Empirical parameters are in orange . | | | | | | | |
| $\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot \left[N_{\text{TECH}} \cdot \sum_i \frac{\text{wt}\%_i \cdot \text{YSI}_i}{VP_i^{\alpha=f(\text{EtOH})}} \right]^{(1 + \beta \cdot (99.9 - \text{FuelCoverage}_{\text{DHA}}))}$ $\alpha = \{ \alpha_{\text{E0}}, \alpha_{\text{E10}}, \alpha_{\text{E20}} \}$ $f(\text{EtOH}) = \alpha_{\text{E0}} + \Delta\alpha \cdot \text{EtOH}_{\text{VOL}\%}$ $\text{FuelCoverage}_{\text{DHA}} = \text{Total Wt\% Identified in DHA}$ $\text{LHV} = \text{Lower Heating Value}$ | | | | | | | |
| 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:

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

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 PMI².

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.

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

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

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 $y\text{Term}_i$ 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 1.00³. 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 D6730-21 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 $1 + \text{DBE}$ 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 estimating⁴ 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/VP α 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.

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

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 $(1 - 0.10) \cdot 1.036 = 0.93$ 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:

$$PM_{i,k} = A_k \cdot PME_i = A_k \cdot \left(\frac{43.4}{LHV} \right) \cdot \left[N_{TECH} \cdot \sum_i \frac{wt\%_i \cdot yTerm_i}{VP_i^{\alpha=\alpha_0+\Delta\alpha \cdot EtOH_{vol\%}}} \right]^1 \quad (2-4)$$

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. | $1/VP^a$ 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. | $1/VP^a$ 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. <i>CRC Project RW-107-3: Validation of the New PM Index Formula.</i> 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. <i>CRC Project RW-107-3: Validation of the New PM Index Formula.</i> 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 |
| <i>Source: Yang 2019a. Table S1, Supplementary Material</i> | | | | | |

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

| Property | Match Blended | | | | | Certification Fuel plus Ethanol Splash Blending | | |
|---|---------------|--------|--------|--------|--------|---|-------------------------------|-------------------------------|
| | Fuel 1 | Fuel 2 | Fuel 4 | Fuel 6 | Fuel 7 | Fuel 3 Tier 3 Cert Fuel | Fuel 5 -> E15 Splash | Fuel 8 -> 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 |
| <i>Source: Yang 2019a. Table 1. Physicochemical properties of the test fuels.</i> | | | | | | | | |

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.

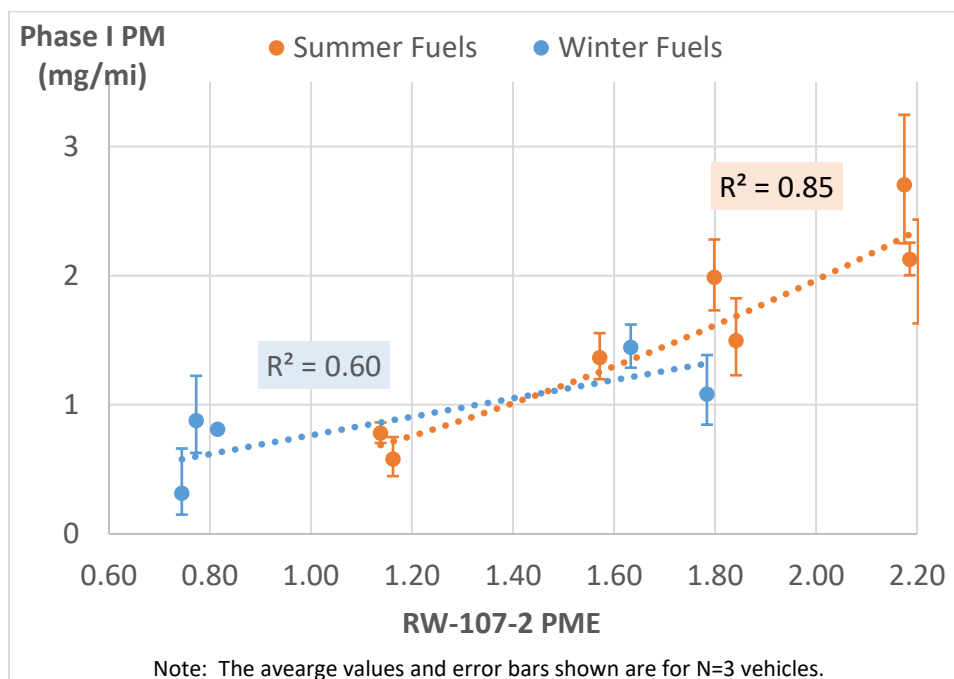
Both the SWRI and Growth Energy datasets passed the due diligence tests without concern. No cause was found to reject any of their data points as outliers, nor was evidence found of test cell drift or vehicle drift. The only quality difference detected between them was that the CE-CERT testing for Growth 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)



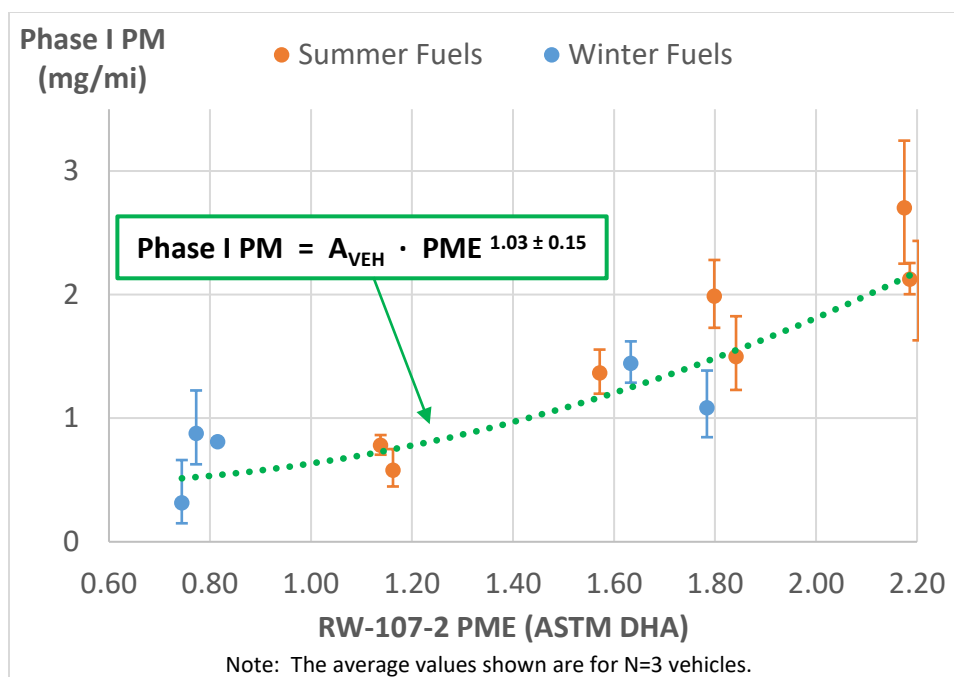
The resolution of Phase I PM measurements at the SwRI laboratory is ~0.25 mg/mi, which suggests that discrimination of PM values should be possible even below 1.0 mg/mi. MSS (micro soot sensor) measurements were examined to confirm this. MSS can be measured at very high resolution, but it represents 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: $\log(\text{Ph I Phase I PM}) = A + B \cdot \text{PME}$. 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 I Phase 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



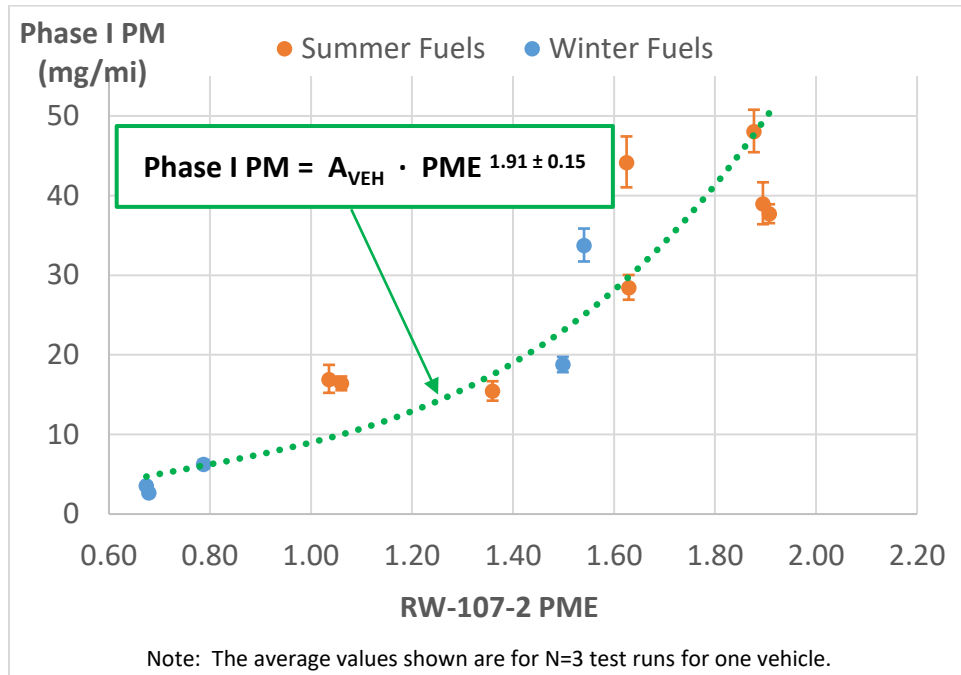
With regard to SIDI vehicles, little can be said based on the SWRI dataset because it contains only a single direct-injection vehicle. Any trend observed in the data pertains only to the individual vehicle and cannot be generalized to other SIDI vehicles as a group. For the SIDI vehicle, the dataset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

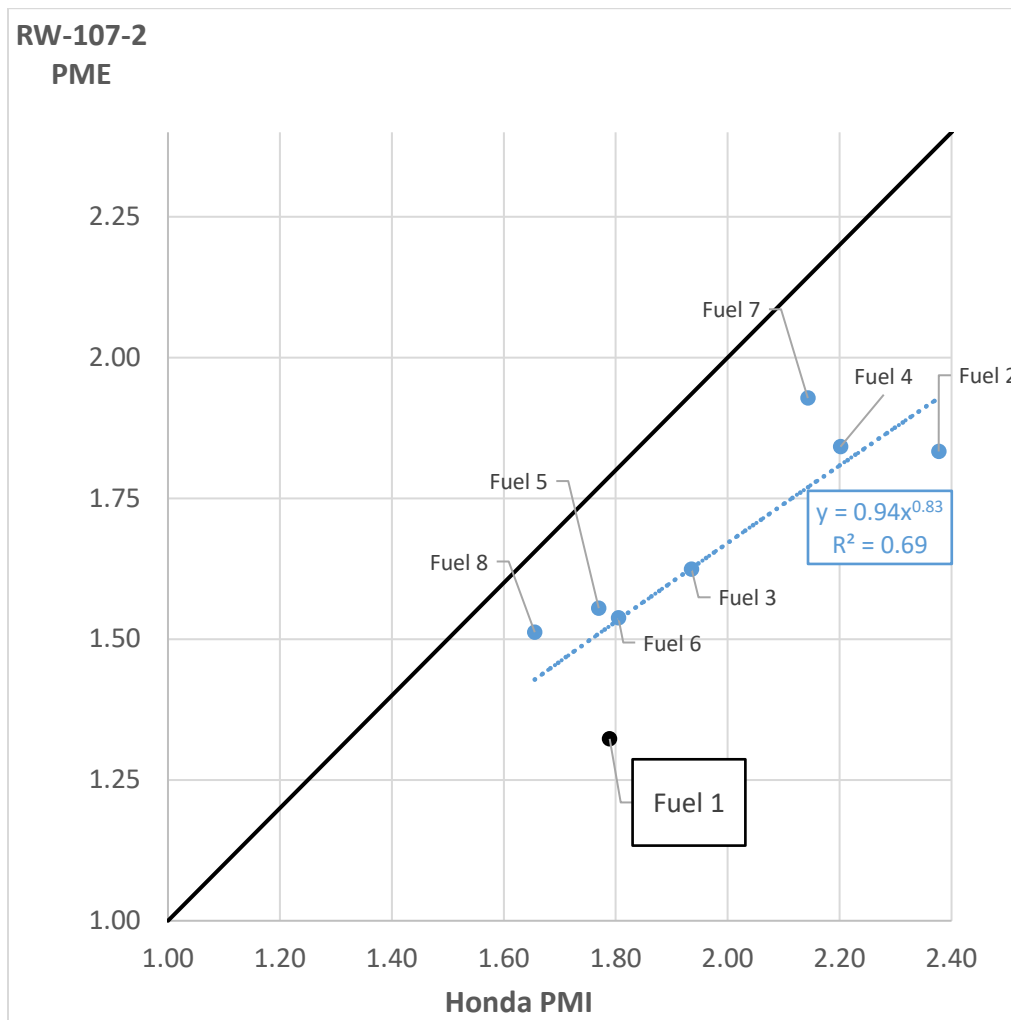
3.4.1 PME Performance Overall

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



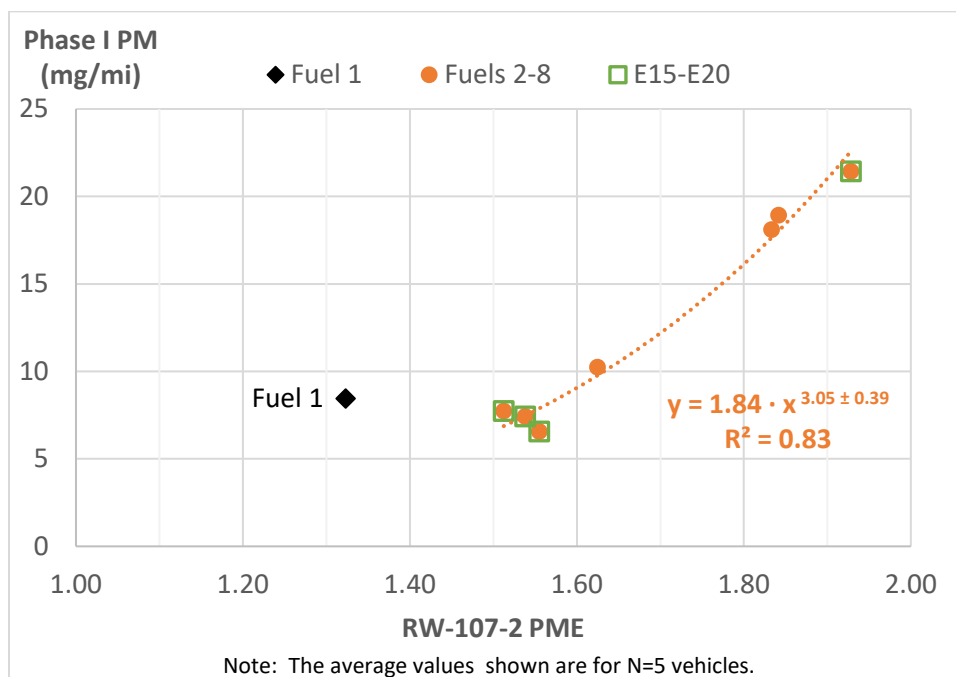
The Fuel 1 discrepancy becomes clearer when Phase I PM emissions are plotted against the PME (see Figure 3-5). All of the other fuels cluster closely around the orange trendline between Phase I PM and PME. Fuel 1 stands well to the left of the other fuels at its PME value of 1.32; in fact, its PME would 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 (Naphthenes) 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 $\alpha=f(\text{EtOH})$ 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



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:

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

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

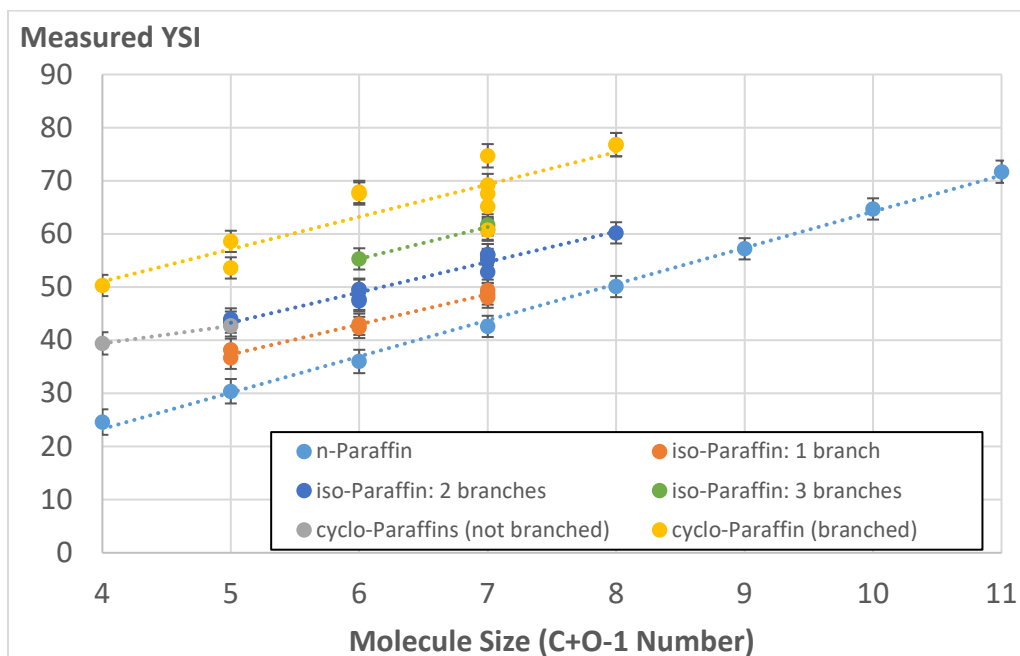
Investigation of the Fuel 3 discrepancy with its high fractions of iso- and cyclic-paraffins led to the discovery that the reality of soot formation in paraffins was more complex. As Figure 3-6 shows, both the type of saturate (whether n-, iso-, or cyclo-paraffin) and the number of branches in non-straight 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? In Tier 3 vehicles? | Yes, by design No. Exponent of 3.05 ± 0.39 | Yes, by design 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 y_{Termi} , 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 EPA's 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.

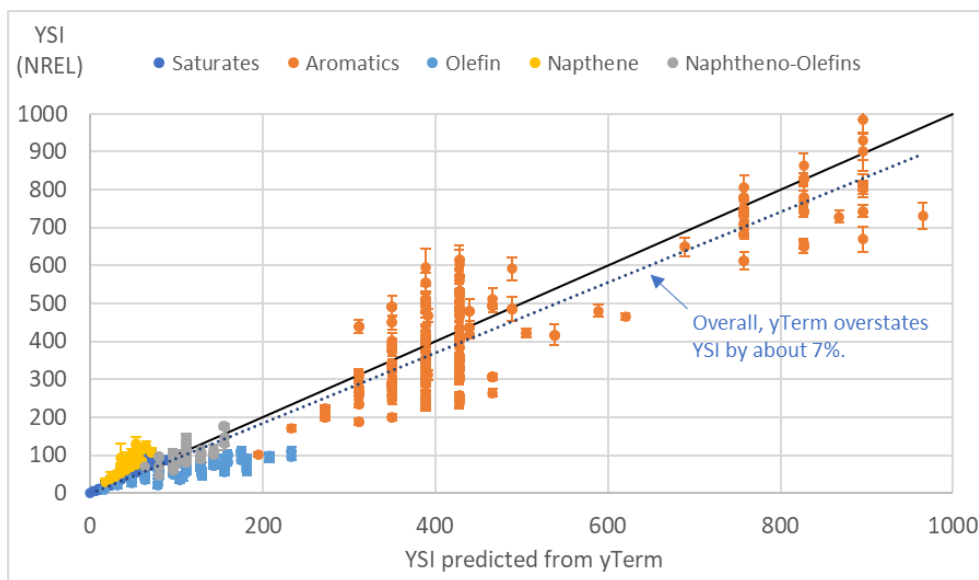
For the CRC database, generic compounds were assigned to the closest eluting compound based on the Retention Indices (RI) that shared the characteristics of the generic entry. The representative compound was then used to determine the YSI value. For the Honda PMI, the representative approach is not needed 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_{443K}) 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 EPAAct, 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 calculator⁵ 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 EPAAct 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.

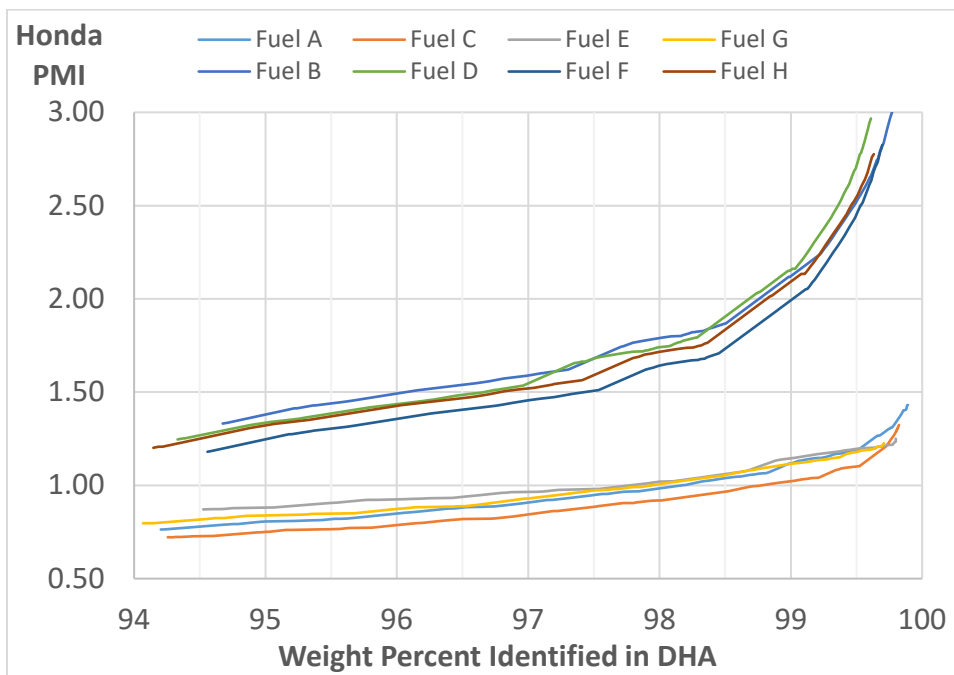
To address this need, the SSI DHAs for the E-94-2 experimental gasolines were examined to understand how the index value will change as the wt% coverage increases and to what extent the final index value (meaning at the maximum wt% coverage) can be estimated from an earlier index value at lower wt% coverage.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



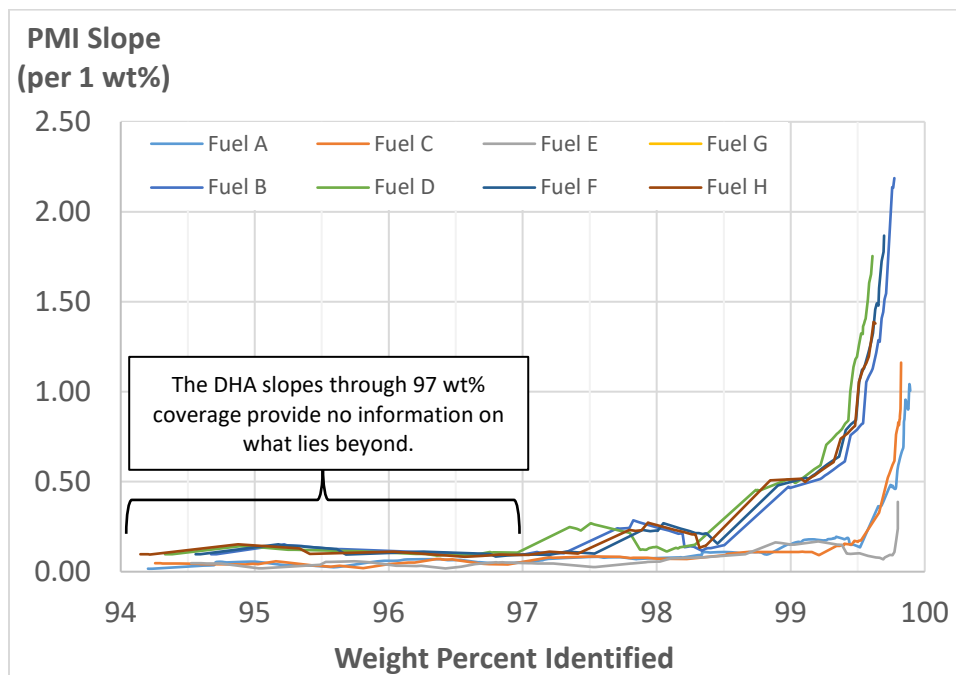
An effort was made using the E-94-2 gasolines to predict the PMI value at the end of the SSI DHA as a function of the wt% coverage and PMI value and slope of the PMI curve at varying points on the DHA. The local slope of the DHA was chosen as a factor that might tailor the expansion of calculated PMI 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 PME 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 the 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.

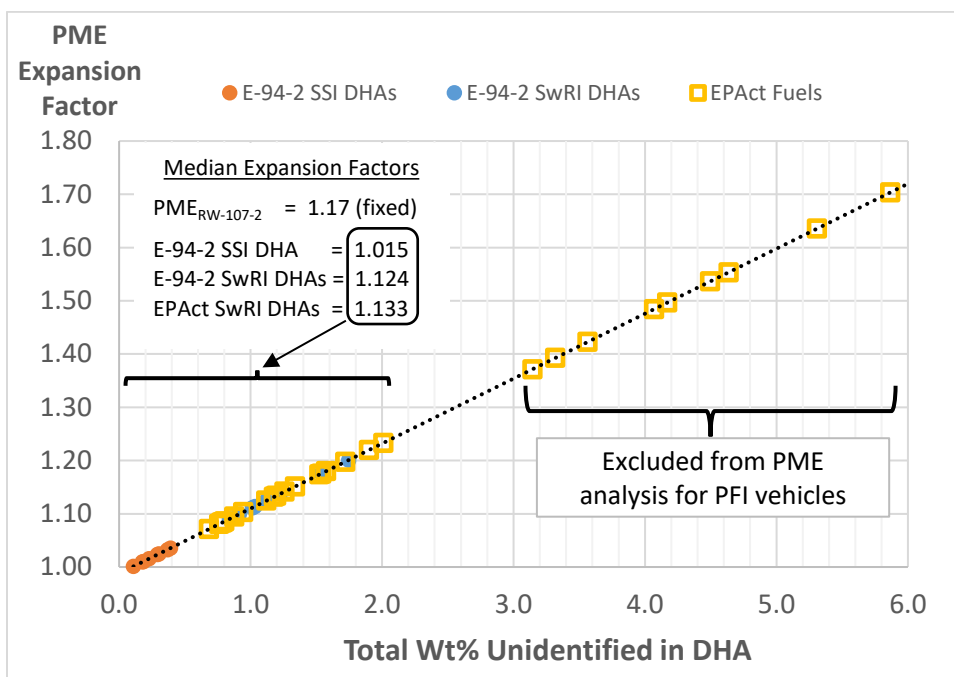
The PME expansion factor β was estimated along with the other empirical coefficients in the analysis of the E-94-2 data where both ASTM and SSI DHAs were available for each gasoline. The mathematical form of the adjustment was:

$$\text{PME}_{99.9} = \text{PME}_{\text{EOC}}^{(1 + 0.122 \cdot \text{UnID})} \quad (4-1)$$

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

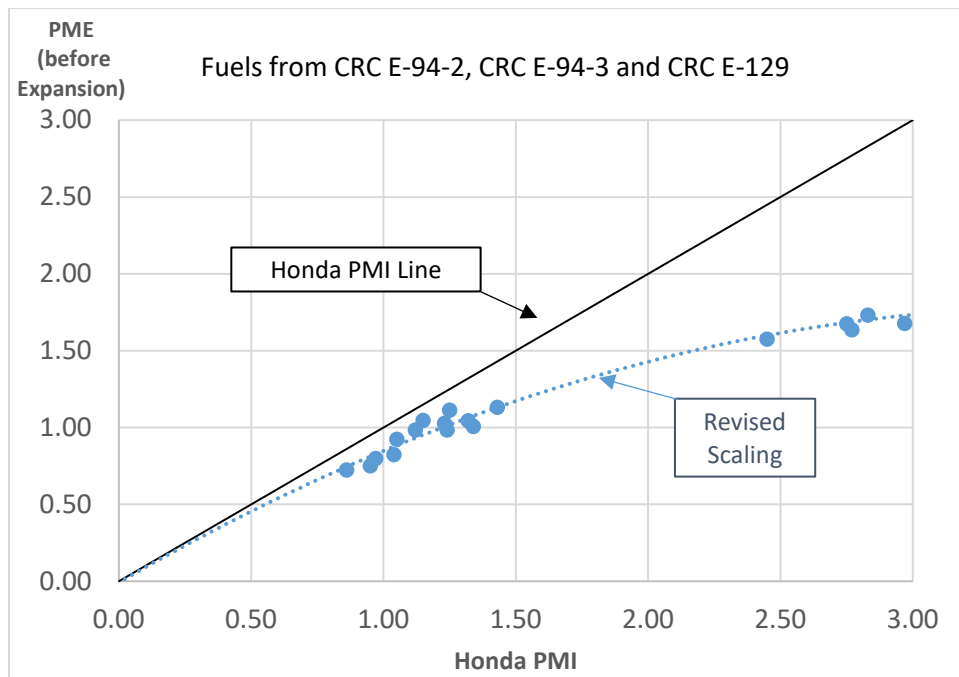
A final revision was made to the methodology for determining PME. The “raw” PME value computed from the summation term in Eq. 1-2 can be as high as 100 to 1000. Some form of scaling is needed so that PME can be compared intuitively to Honda PMI values. This implies that the PME value should be close 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 $\{\alpha_{E0}, \alpha_{E10}, \text{ and } \beta\}$ 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 EPAAct dataset of 18 gasolines. A comparable iterative search was then conducted for the set of coefficients $\{\alpha_{E0}, \alpha_{E10}, \text{ and } \alpha_{E20}\}$. 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 EPAAct 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 EPAAct 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 EAct 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 EAct 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.

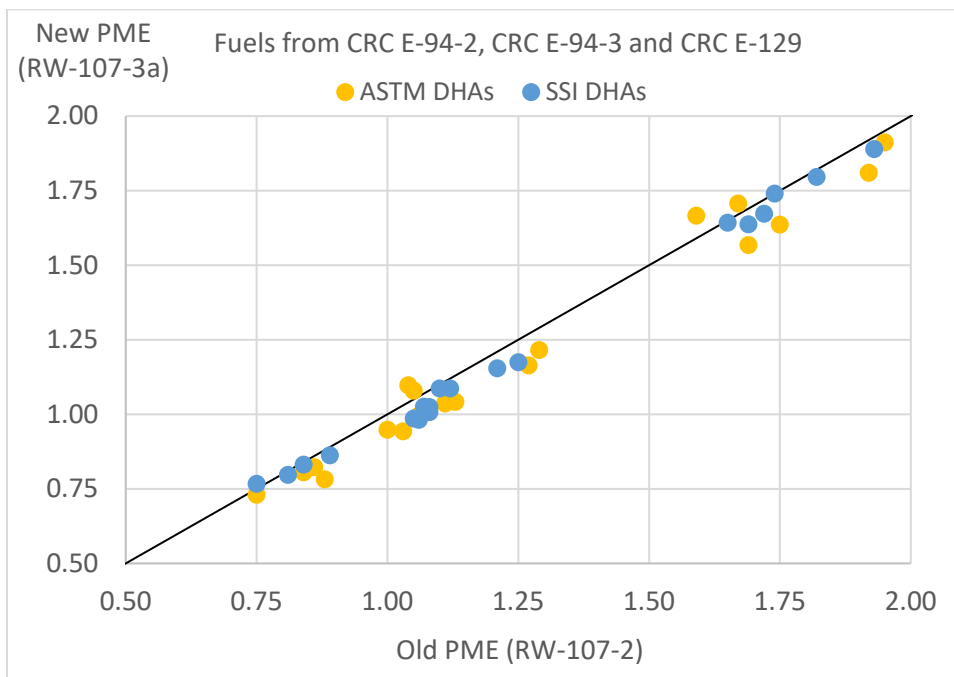
4.7 Comparison of Old and New PME Values

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% ($\beta=1.17$) 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.

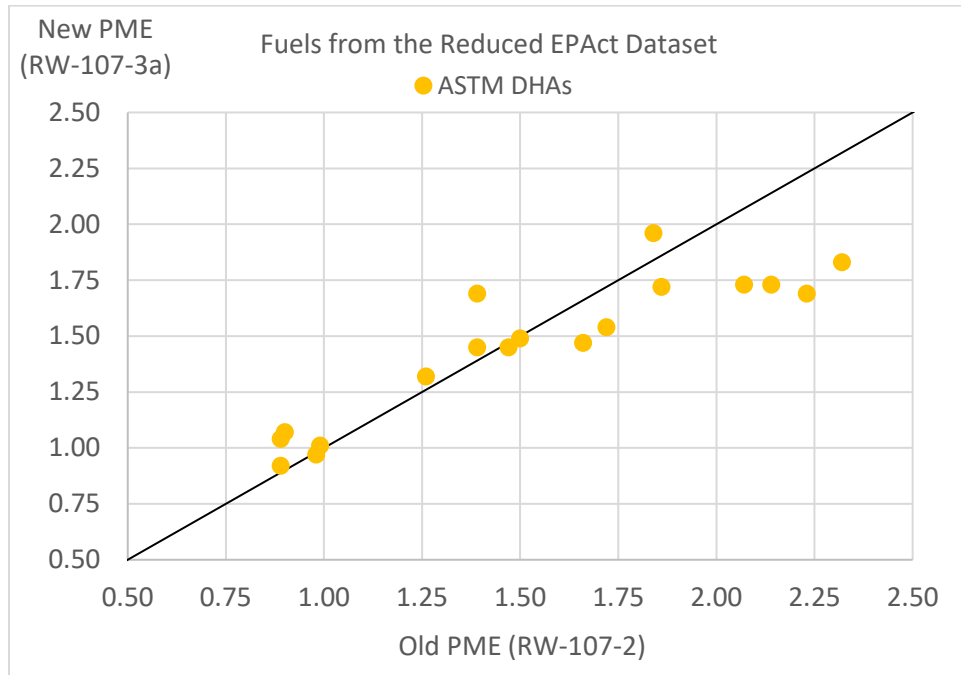
Figure 4-6
Comparison of Old PME and New PME Values for SIDI Vehicles



For PFI vehicles, Figure 4-7 shows that there is good overall correspondence between Old and New PME values for fuels in the Reduced EPAAct 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 EPAAct 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

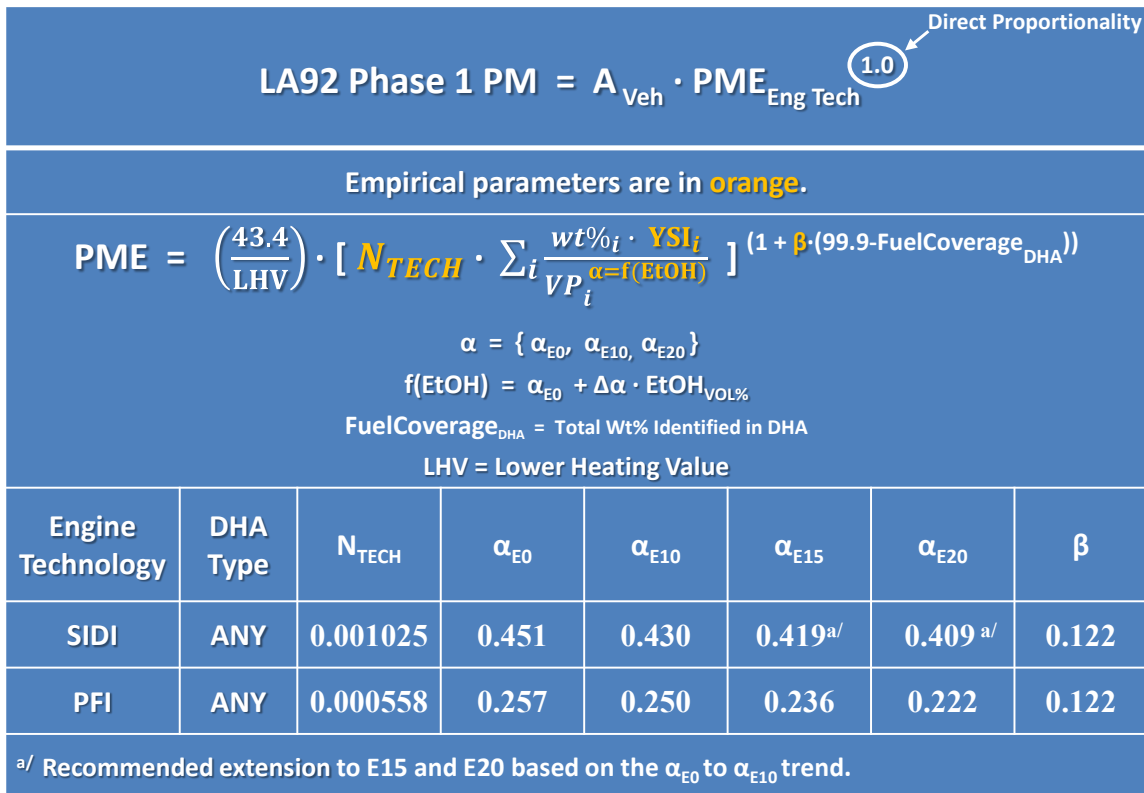


5. THE NEW PME FORMULATION

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



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 all 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 EPA Act, 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).

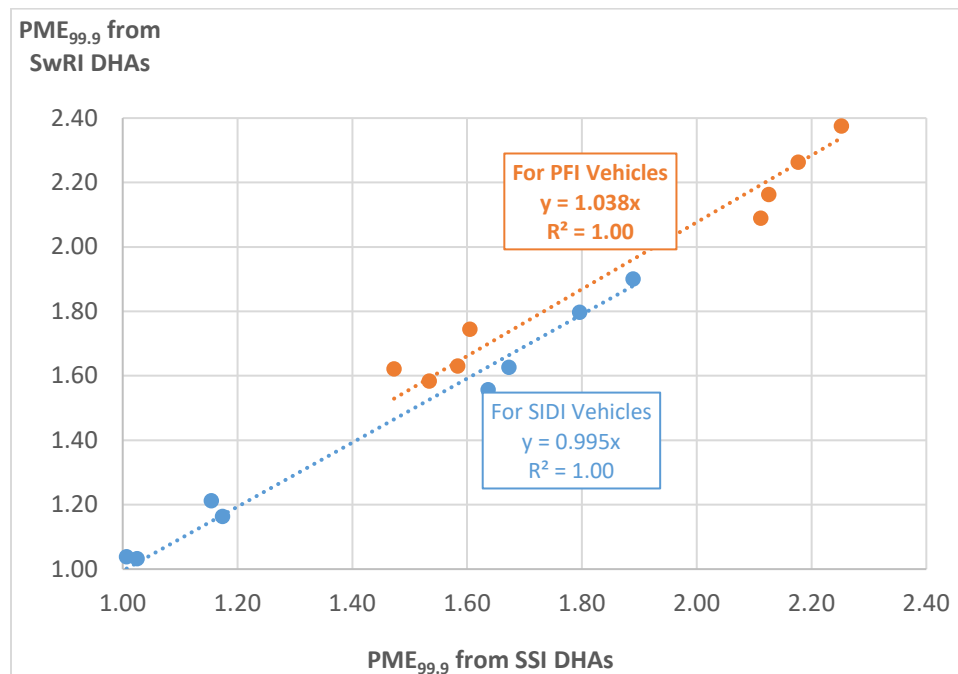
As given in the lower portion of the figure, two sets of empirical coefficients are given for New PME. One set pertains to SIDI vehicles and the other to PFI vehicles. A spreadsheet-based PME calculator is available from CRC that will translate a DHA into two PME index

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 EPAAct 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.

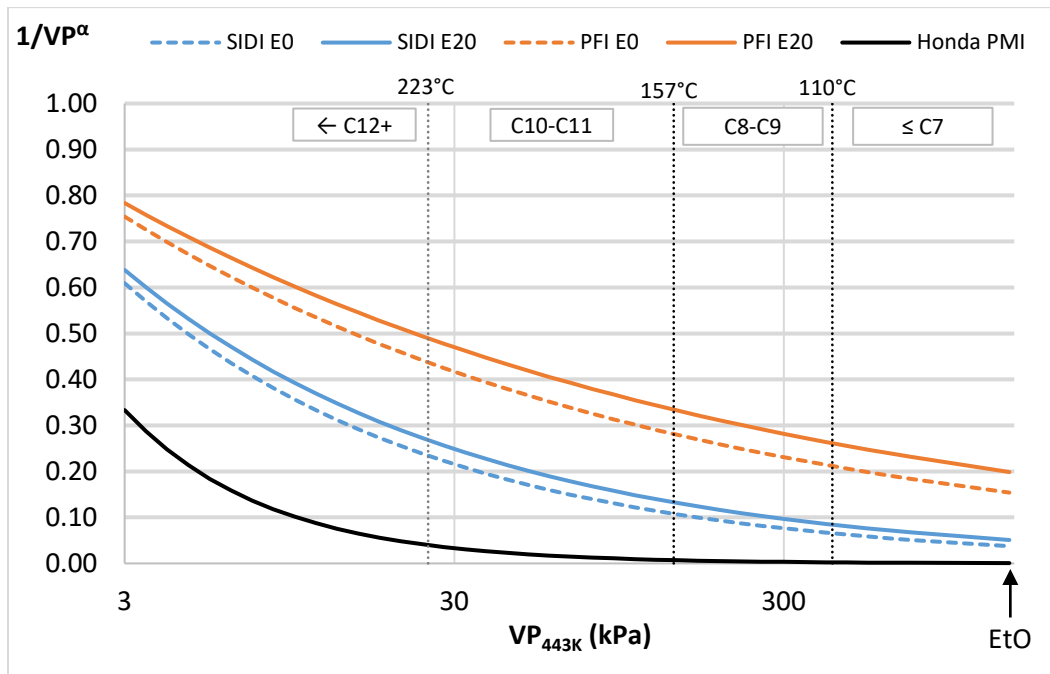
Figure 5-2
Equivalence of Expanded New PMEs from SSI and SwRI DHAs



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 is 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.

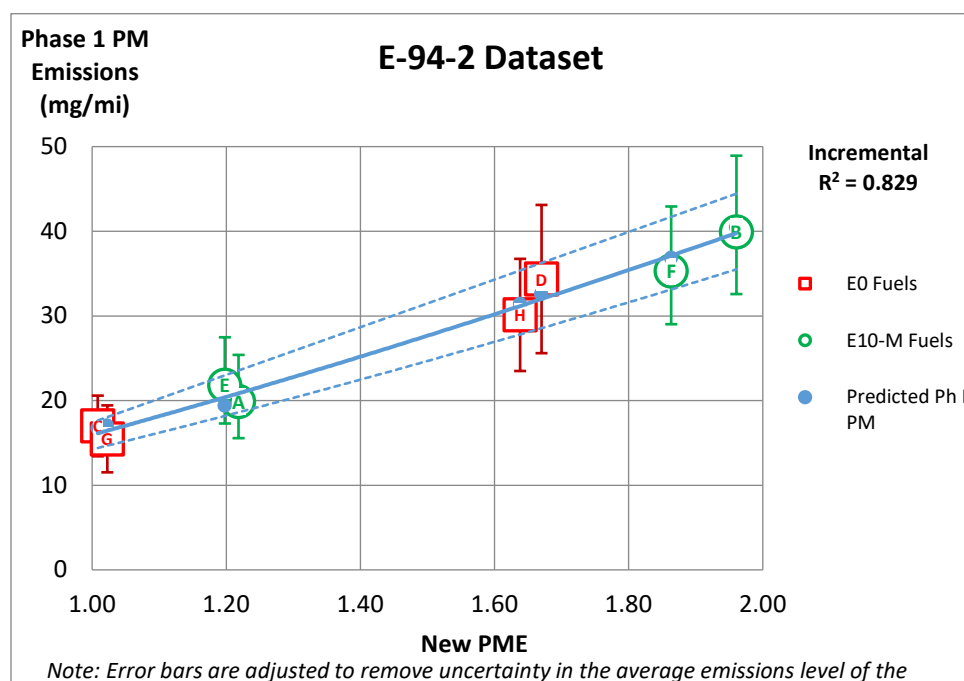
As before, an analysis of the emissions residuals was conducted after the final PME fit to determine whether the bulk properties of the gasolines carried additional explanatory power for PM emissions. RVP and its correlate T05 were found to have a statistically significant relationship to residual emissions, 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



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-A⁸ 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.
- ρ_{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 |
| rPEARSON | 0.99 | | n/a |
| ρSPEARMAN | 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

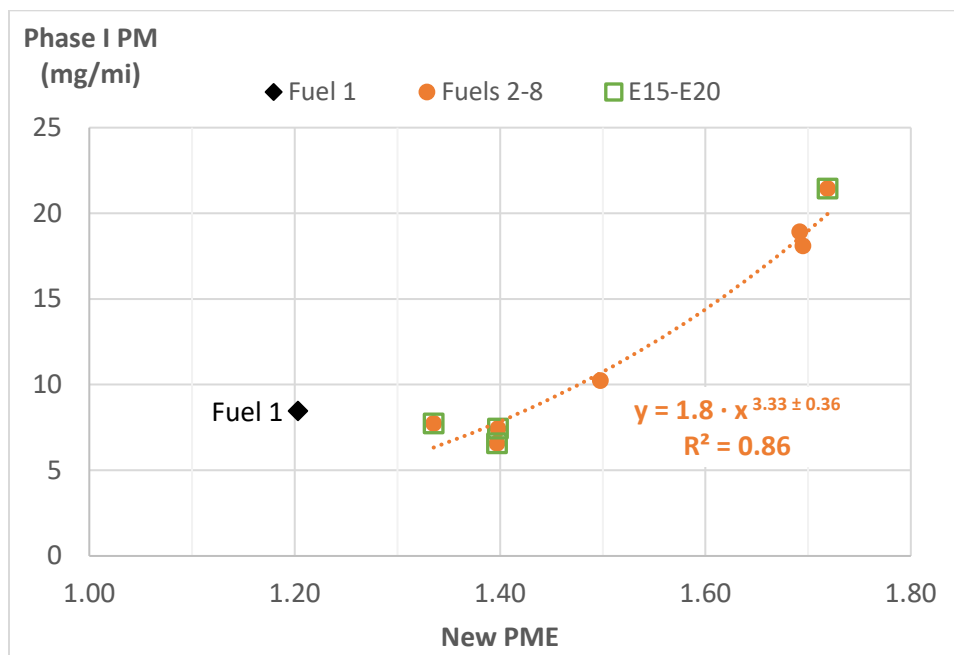
MAE errors approximately nearly one-half that of PMI, and is without ethanol bias. In contrast, PMI has an ethanol bias that ranges from 11 to 22%. The New PME is a large improvement over PMI.

The high r_{PEARSON} and ρ_{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 EPAAct dataset used here very different from the complete EPAAct 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 EPAAct Dataset

Figure 5-6 shows the performance of New PME as a predictor of LA92 Phase I PM emissions in the reduced EPAAct 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 EPAAct 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 EPAAct dataset than did the Old PME in the complete EPAAct dataset (see corresponding Figure 6-3 of the RW-107-2 report). Its high r_{PEARSON} and ρ_{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

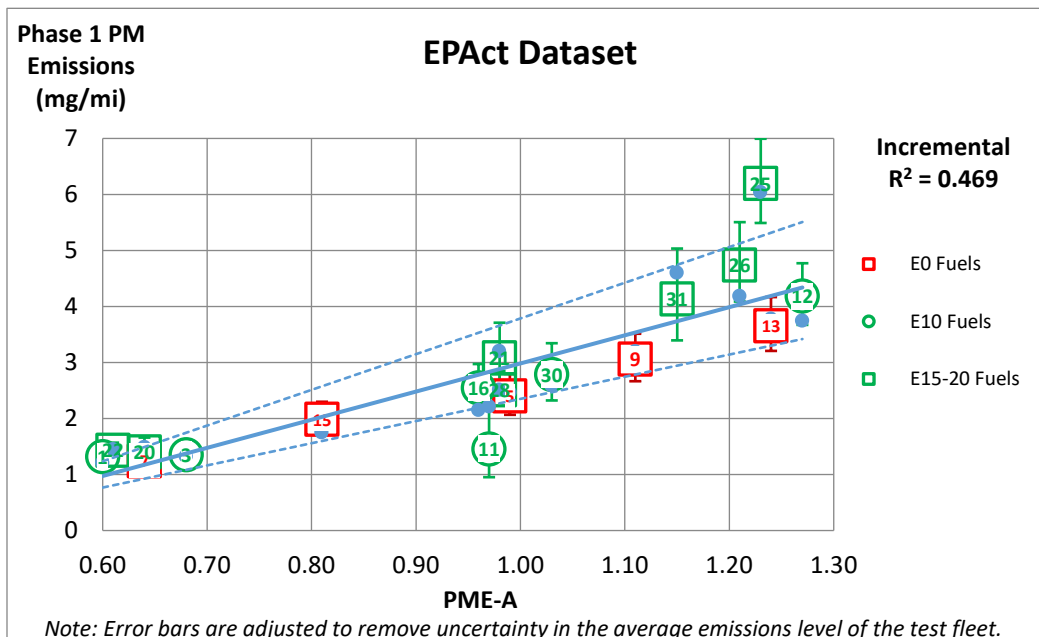


Table 5-2
New PME Performance Measures for the Reduced EPAct Dataset

| | New PME This Study | | Honda PMI* RW-107 |
|--|-----------------------|---------|----------------------|
| Incremental R ² | 0.469 | | 0.394 |
| r _{PEARSON} | 0.94 | | n/a |
| ρ _{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

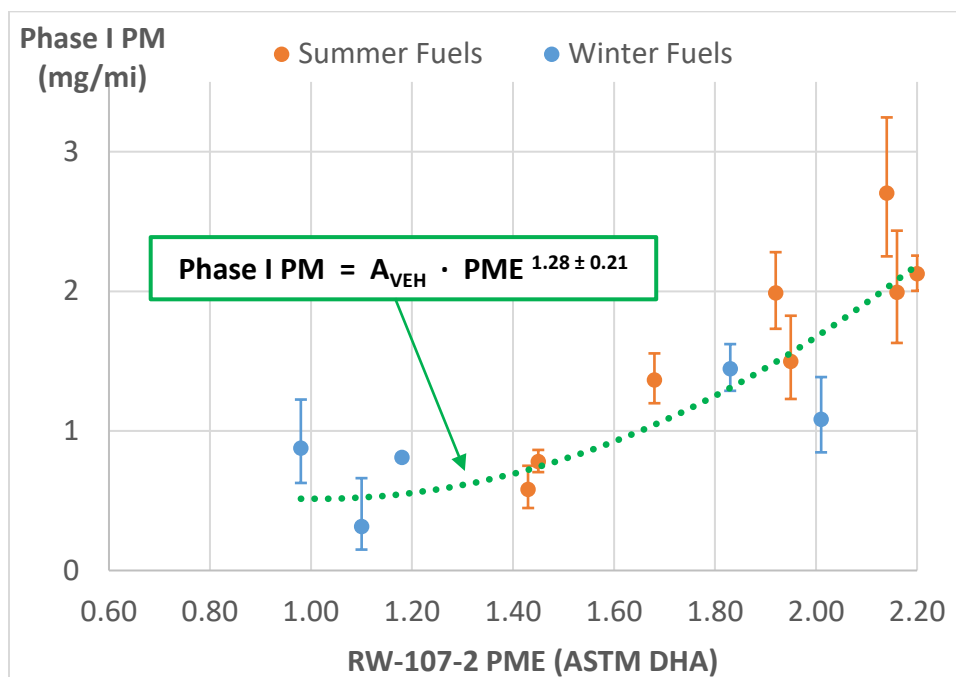
statistically significant) is greatly strengthened with the New PME in which no ethanol bias is present. The New PME for PFI vehicles is a clear-cut improvement over the Old PME.

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/mi⁹. 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.

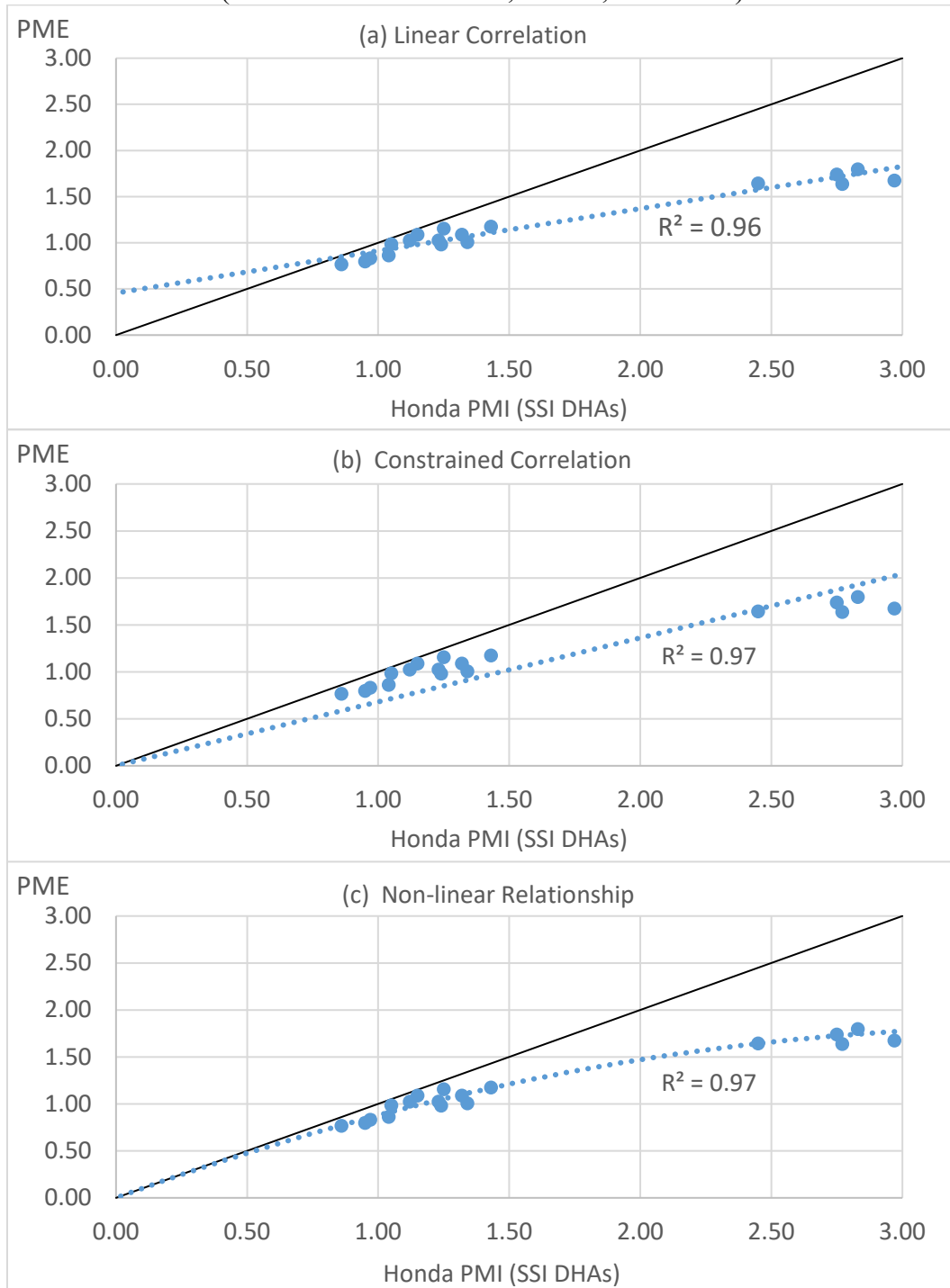
6.1 The Relationship of the PM Indices

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 $r \sim 0.98$ 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 ($\text{DBE} = 0$) in order to give a zero or near-zero PMI value¹⁰. 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 footnote¹¹) 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.

¹⁰ An entirely paraffinic gasoline would have a PMI index value of $1/\text{VP}$, 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:

$$\text{Phase I PM}_{i,k} = A_k \cdot \text{PME}_i^{1.0} \quad (6-1)$$

$$\log(\text{Phase I PM}_{i,k}) = \log(A_k) + 1.0 \cdot \text{PME}_i \quad (6-2)$$

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.

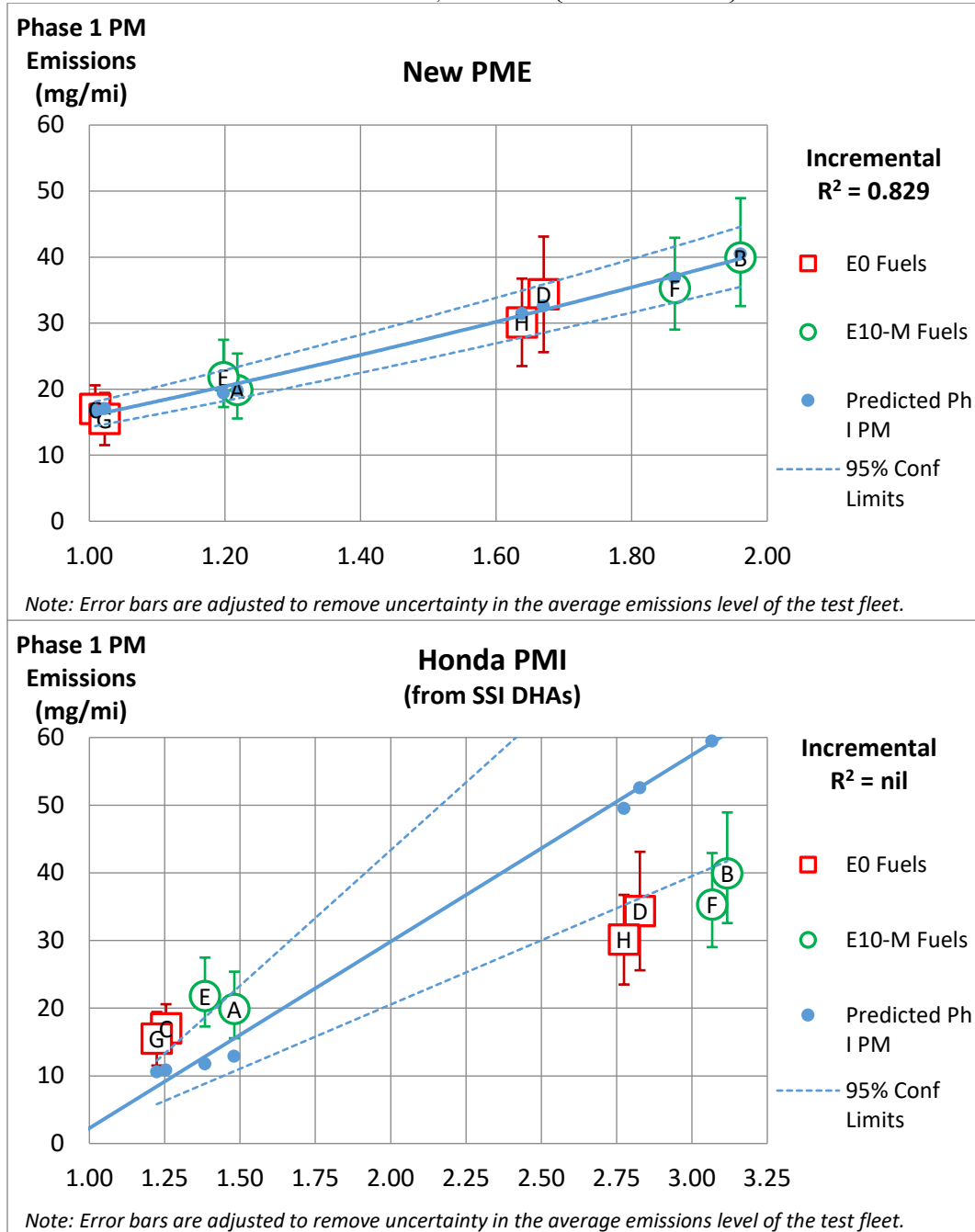
Unlike most regression analysis, the coefficient takes on a fixed value of 1.0 to indicate the direct proportionality of the index to emissions, rather than a variable value that is determined empirically in the regression fit. While unlike most models, these can be fit by a non-linear regression method 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 EPAAct 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

$$\text{LA92 Phase I PM}_{i,k} = A_k \cdot \{\text{PME}_i \text{ or PMI}_i\}^{1.0}$$



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 $R^2 = 0.829$ value¹² 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.

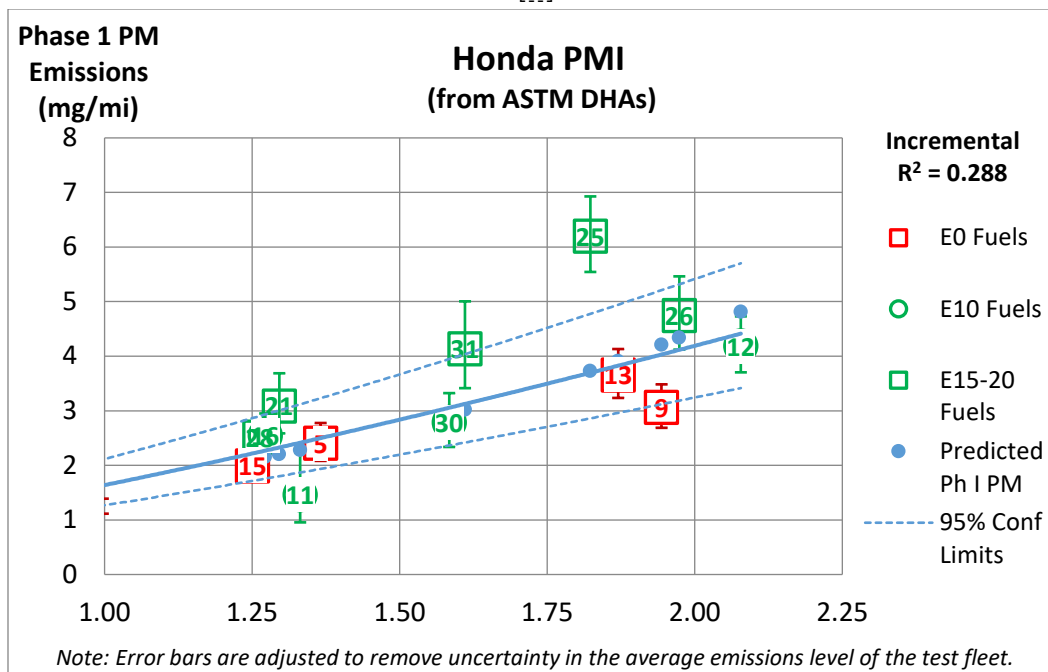
Figure 6-3 presents similar graphs that apply the New PME and Honda PMI to the data of the Reduced EPAAct dataset (PFI vehicles). The upper portion shows the performance of the New PME and was previously seen in Figure 5-6. The data points cluster closely around the overall trendline (with one exception), 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

$$\text{LA92 Phase I PM}_{i,k} = A_k \cdot \{\text{PME}_i \text{ or } \text{PMI}_i\}^{1.0}$$



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.
- ρ_{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 EPAAct 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 ρ_{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 EPAAct 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 ρ_{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

$$\text{LA92 Phase I PM}_{i,k} = A_k \cdot \{ \text{PME}_i, \text{PMI}_i \}^{1.0}$$

| | New PME | | Honda PMI* | |
|--|---------|---------|------------|---------|
| Incremental R ² | 0.829 | | None | |
| rPEARSON | 0.99 | | 0.96 | |
| ρSPEARMAN | 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

$$\text{LA92 Phase I PM}_{i,k} = A_k \cdot \{ \text{PME}_i, \text{PMI}_i \}^{1.0}$$

| | New PME | | Honda PMI* | |
|--|---------|---------|------------|----------|
| Incremental R ² | 0.469 | | 0.288 | |
| r _{PEARSON} | 0.94 | | 0.83 | |
| ρ _{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 figure¹³. 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.

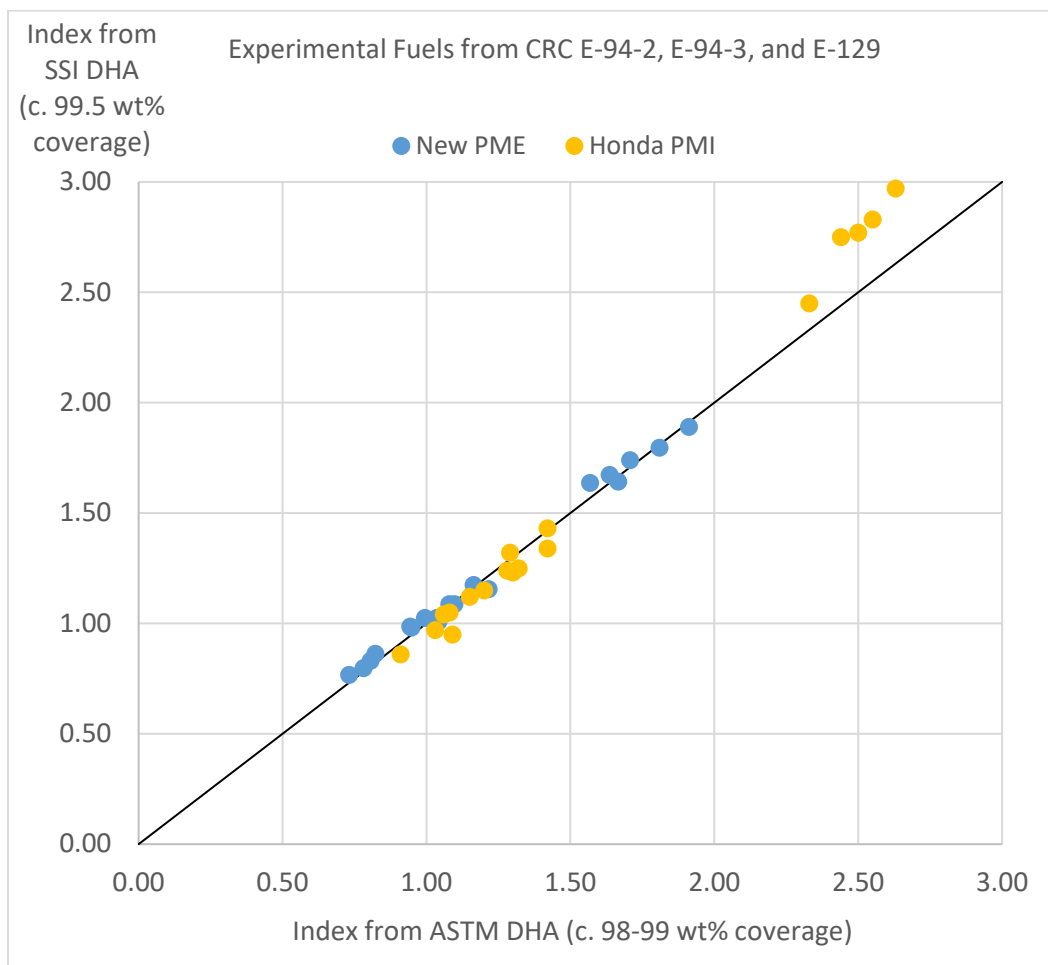
As is apparent, the New PME index values in blue cluster closely along the line of equality. This is because the index value is standardized during its calculation to the value that would be expected at a constant reference coverage of 99.9 wt%. By design, the New PME values are invariant with respect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

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.

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.

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 $\pm 20\%$ 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

| $\text{LA92 Phase 1 PM} = A_{\text{Veh}} \cdot \text{PME}_{\text{Eng Tech}} \quad \text{Direct Proportionality} \quad \text{1.0}$ | | | | | | | |
|---|----------|-------------------|-----------------|------------------|---------------------|---------------------|-------|
| Empirical parameters are in orange . | | | | | | | |
| $\text{PME} = \left(\frac{43.4}{\text{LHV}} \right) \cdot \left[N_{\text{TECH}} \cdot \sum_i \frac{\text{wt}\%_i \cdot \text{YSI}_i}{V P_i^{\alpha=f(\text{EtOH})}} \right] (1 + \beta \cdot (99.9 - \text{FuelCoverage}_{\text{DHA}}))$ $\alpha = \{ \alpha_{\text{E0}}, \alpha_{\text{E10}}, \alpha_{\text{E20}} \}$ $f(\text{EtOH}) = \alpha_{\text{E0}} + \Delta\alpha \cdot \text{EtOH}_{\text{VOL}\%}$ $\text{FuelCoverage}_{\text{DHA}} = \text{Total Wt\% Identified in DHA}$ $\text{LHV} = \text{Lower Heating Value}$ | | | | | | | |
| 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

CRC Report No. RW-107-3

Validation of the New PM Index Formula: Vehicle Testing Phase

Final Report

April 2023



COORDINATING RESEARCH COUNCIL, INC.
5755 NORTH POINT PARKWAY • SUITE 265 • ALPHARETTA, GA 30022

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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
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Attention: Amber Leland**

April 2023

POWERTRAIN ENGINEERING DIVISION

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Final Report

Validation of the New PM Index Formula: Vehicle Testing Phase Project RW-107-3

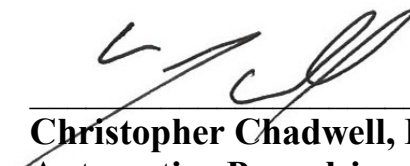
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Southwest Research Institute® Final Report

April 2023

FOREWORD

This report covers testing conducted by Southwest Research Institute (SwRI) for Coordinating Research Council (CRC). The Project, performed under CRC contract RW-107-3, was performed between October of 2020 and February of 2022. The project was based on SwRI's technical proposal to CRC dated October 13, 2020. The internal SwRI project number was 03.26322. The CRC project oversight was led by Amber Leland. The SwRI project manager was Matt Blanks, assisted in testing and development by Peter Lobato and Michael Kader. Laboratory emissions testing were overseen by David Zamarripa. Tim Martinez was the driver for all tests and Kevin Hohn operated the chassis dynamometer and laboratory emissions equipment for this project. All fuel-related and mileage accumulation tasks were managed by Kevin Brunner. This report provides the basic test results and documents the technical effort required to collect the data. Statistical conclusions relating test results to fuel PMI are given in the CRC report for Project RW-107-3a, prepared under a separate CRC contract with Rincon Ranch Consulting, and are not presented in this report.



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1.0 EXECUTIVE SUMMARY

This report documents a project conducted by Southwest Research Institute (SwRI) on behalf of Coordinating Research Council (CRC). The project investigated exhaust particulate emissions from a matrix of vehicles and fuels to validate a new Particulate Matter Index (PMI) formula. This project was conducted in parallel with CRC Projects E-122-2 and E-133 to take advantage of commonalities. LA92 Phase 1 emissions were collected during those projects and are presented in this report. This project was not designed as a stand-alone project; the objective was to provide a fresh, independent dataset for the purpose of validating the new PMI formula developed in CRC Project RW-107-2. The PMI formula validation work was performed by Rincon Ranch Consulting under CRC Project RW-107-3a.

This project evaluated exhaust emissions from four light-duty vehicles using thirteen test fuels. Six of the fuels were commercially available market fuels and six of the fuels were produced by splash blending ethanol with a market fuel to produce new E10 and E15 fuels. The last fuel was an emissions-grade certification gasoline. The matrix of fuel-vehicle combinations was evaluated based on the Design Of Experiments (DOE) initially determined under E-122-2 and E-133. Many of the test fuels were also procured under E-122-2 and E-133. With guidance provided by the CRC committee, SwRI oversaw procurement of two new market fuels and two new splash-blended fuels unique to this project.

The four test vehicles were procured under E-122-2. The vehicles were selected to include targeted engine and vehicle technologies. One vehicle was provided by CRC and the other three were procured by SwRI from local dealerships. New vehicles were driven on milage accumulation dynamometers (MADS) to an odometer reading of 4,000 miles. The oil and oil filter were changed on all vehicles and 500 miles was accumulated to de-green the new oil before emission tests were conducted. Results in this report are blinded to vehicle identifications.

Duplicate cold-start LA92 drive cycles were used for each fuel-vehicle combination with a third test conducted if repeatability of the first two tests did not meet predetermined criteria. Approximately 144 cold-start chassis dynamometer emission tests were conducted for this project. Figure 1 shows vehicle particulate mass (PM) emissions compared to the fuel PMI value. All vehicles gave an increasing trend in particulate mass with increasing fuel PMI, although, statistical analysis was not conducted to evaluate significance of the trends.

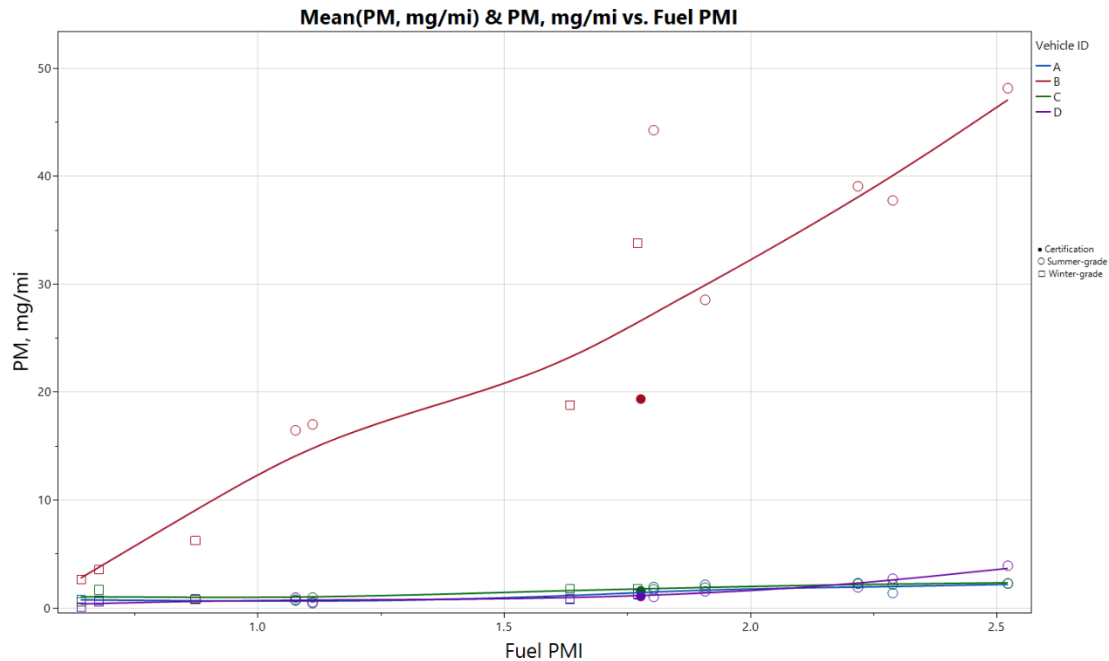


FIGURE 1. LA92 PHASE 1, PM EMISSIONS VS FUEL PMI

2.0 INTRODUCTION

A previous CRC Project, RW-107, revealed that the original Particulate Matter Index (PMI) exhibited an ethanol bias. A more robust PMI formulation was developed in CRC project RW-107-2, in which correlation with measured PM was improved, and the ethanol bias eliminated. The new formulation incorporated multiple enhancements. A fresh dataset is required to validate this new form of the PM Index equation, preferably including a range of PMI values, vehicle technologies, and fuel formulations. The project was initiated on October 20, 2020 and official testing began on October 28, 2020. Testing with the final fuel concluded over two years later, January 17, 2022.

3.0 PROJECT SETUP

All tests were conducted at SwRI's light-duty vehicle laboratory. Tim Martinez was the driver and Kevin Hohn operated the test facility and laboratory emissions equipment for the entire project. The following sections detail test fuels, test vehicles, and the emission test procedure.

3.1 Test Fuels

Five of the test fuels were located and procured under CRC Project E-122-2. Four of these fuels were market fuels, comprised of summer and winter grades, each having a low and high Particulate Matter Index (PMI). For this project, a PMI rating of 1.0 was considered low and a rating of 2.0 was considered high. Although not all collinearities in fuel properties were investigated, PMI was highly correlated with back-end distillation (especially final boiling point). Thus, trends observed in this data for a response variable (such as PM emissions) over the range of PMI investigated may be due to PMI, or to one or more other correlated properties.

Emissions-grade certification fuel was also procured from Haltermann Solutions under that project. All market fuels were 87 Anti-Knock Index (AKI) E10 regular unleaded (RUL), except for the winter-grade, high PMI fuel. This fuel was a 93 AKI E10 premium unleaded (PUL), because a RUL winter-grade fuel, meeting the Reid Vapor Pressure (RVP) and PMI requirements, could not be located. The PUL fuel was supplied by a major refiner unadditized but was additized at the minimum TOP TIER® treat rate before use. The four E10 market fuels were then splash blended with ethanol to E15, under CRC Project E-133, to give nine initial fuels. Acquisition of these market fuels occurred over a one-year period since no winter fuels of the desired PMI level were located within the 2020 high vapor pressure season.

With assistance from CRC members, two new fuels were identified and procured specifically for this project. The first was a summer-grade, high PMI E0, that was procured from a CRC member refinery terminal. The second was a winter-grade, low PMI E0, that was procured from a different CRC member refinery terminal. Each of these E0 fuels were RUL with an AKI of 88. SwRI arranged to transport these fuels using a tanker truck that was steam-cleaned, dried, and inspected before being sealed and dispatched to acquire the fuel. Figure 1 shows examples of seals installed on a tanker truck after being inspected by SwRI. Upon arrival at SwRI, a sample of each fuel was drawn from the tanker and analyzed for key fuel properties. After approval, the fuel was offloaded into pre-inspected epoxy-phenolic lined drums and stored at 70 °F. Portions of the summer-grade, high PMI E0 were then splash blended to make both an E10 and an E15 test fuel. Results of the key properties from each fuel are shown in Table 1. Fuels J, K, L, and M are the fuels acquired specifically for this project. Detailed analysis results and a full description of the fuel procurement process are given in Appendix A.

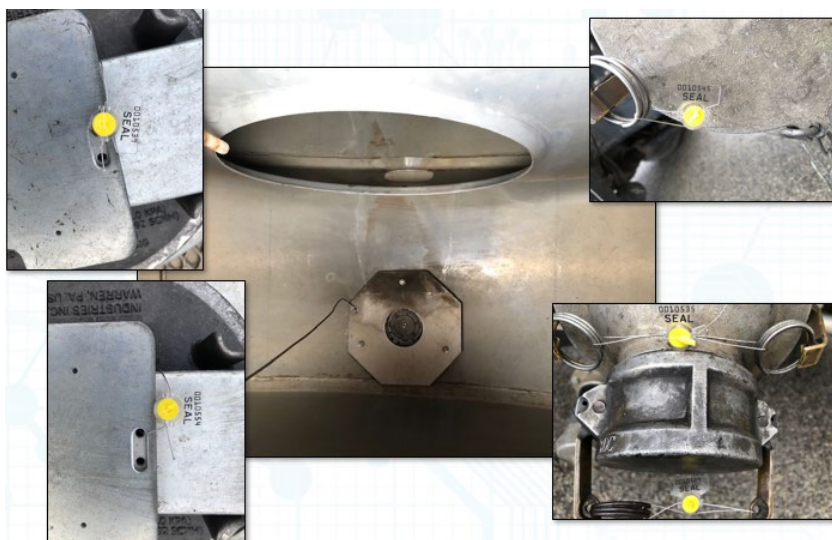


FIGURE 2. FUEL TANKER INSPECTION AND SEALS

TABLE 1. ANALYSIS RESULTS OF KEY FUEL PROPERTIES

| ID | Code | Description | Ethanol, vol% (ASTM D4815 / D5599) | PMI (ASTM D6729) | RVP, PSI (ASTM D5191) | FBP, °F (ASTM D86) | Total Aromatics, Wt% (ASTM D6729) | Notes |
|----|-----------|---------------------|---------------------------------------|---------------------|--------------------------|-----------------------|--------------------------------------|-------------------------------|
| A | EM-10967 | Certification E10 | 9.7 | 1.8 | 9.2 | 388 | 27.6 | EPA Tier 3 EEE |
| B | GA-10940 | Summer Low PMI E10 | 9.7 | 1.1 | 9.0 | 367 | 24.4 | |
| C | GA-10920 | Summer High PMI E10 | 9.5 | 1.9 | 7.7 | 408 | 33.2 | |
| D | GA-11027 | Winter Low PMI E10 | 9.6 | 0.7 | 15.3 | 344 | 25.8 | |
| E | CGB-11093 | Winter High PMI E10 | 10.2 | 1.8 | 13.6 | 392 | 32.7 | PUL |
| F | CGB-11037 | Summer Low PMI E15 | 15.2 | 1.1 | 8.8 | 373 | 23.8 | Fuel B + Ethanol Splash Blend |
| G | CGB-11039 | Summer High PMI E15 | 15.0 | 1.8 | 7.6 | 395 | 31.9 | Fuel C + Ethanol Splash Blend |
| H | CGB-11156 | Winter Low PMI E15 | 15.3 | 0.6 | 14.2 | 344 | 17.3 | Fuel D + Ethanol Splash Blend |
| I | CGB-11149 | Winter High PMI E15 | 15.3 | 1.6 | 13.3 | 396 | 30.2 | Fuel E + Ethanol Splash Blend |
| J | GA-10950 | Summer High PMI E0 | <0.2 | 2.5 | 8.7 | 427 | 43.1 | |
| K | GA-11026 | Winter Low PMI E0 | <0.2 | 0.9 | 14.5 | 361 | 26.1 | |
| L | CGB-11147 | Summer High PMI E10 | 10.1 | 2.3 | 9.4 | 417 | 38.8 | Fuel J + Ethanol Splash Blend |
| M | CGB-11148 | Summer High PMI E15 | 15.1 | 2.2 | 9.4 | 421 | 37.2 | Fuel J + Ethanol Splash Blend |

3.2 Test Vehicles

Four vehicles were used in this project. CRC supplied one vehicle and SwRI purchased the other vehicles from local dealerships under CRC Project E-122-2. Table 2 gives a description of each vehicle listing key properties that were targeted for each selection. These technologies include Port Fuel Injection (PFI), Direct Injection (DI), turbo charging, electric hybrid, and engine Start/Stop.

Along with vehicle descriptions, this section discusses vehicle-specific topics that include the following:

- Tasks performed with each vehicle after purchase
- Initial checkout tests and results
- Problems encountered with individual vehicles while testing

TABLE 2. TEST VEHICLES

| Test ID | A | B | C | D |
|-----------------------------|--------------------------------|------------------|------------------|------------------|
| Year | 2019 | 2013 | 2019 | 2019 |
| Engine Type | PFI NA | DI Turbo | PFI NA | PFI NA |
| Transmission | 6-Speed AT | 6-Speed AT | 9-Speed AT | e-CVT |
| Fuel Type | Premium Gasoline (recommended) | Regular Gasoline | Regular Gasoline | Regular Gasoline |
| Flex Fuel | No | No | No | No |
| Start/Stop | No | No | Yes | Hybrid |
| EPA Cert | T3B125 LDV | T2B5 LDV | T3B30 LDT | T3B30 LDV |
| CA Cert | ULEV125 PC | ULEV II PC | SULEV30 LDT | SULEV30 PC |
| Weight with Empty Tank, lbs | 4,096 | 3,677 | 4,320 | 3,324 |

After purchase, the following tasks were performed with each vehicle.

- Each vehicle was added to SwRI's test vehicle insurance policy
- New vehicles were driven to a 4,000-mile odometer reading on a chassis dynamometer using the US EPA Standard Road Cycle (SRC) drive profile and E10 RUL gasoline
- The oil was changed and 500 miles of the SRC was accumulated for oil degreening using RUL E10 gasoline
- Reports were run to check for powertrain recalls, TSBs (Technical Service Bulletins), DTCs (Diagnostic Trouble Codes), and required vehicle software updates
- The coolant freeze-point and fill level were checked
- Tires were inspected

3.2.1 Emissions Verification Test

Prior to the start of testing, each vehicle was flushed with certification-grade fuel and tested over a single FTP-75 cycle to determine if the vehicle's emission control system was working properly. Regulated emissions (Non-Methane Hydrocarbons (NMHC), CO, CO₂, NO_x, and PM) were measured and provided to CRC for final approval of the vehicles. All vehicles produced emissions well below their certification level. Table 3 gives the results from each checkout test.

TABLE 3. CHECKOUT EMISSION RESULTS

| | | CO, g/mi | NMOG+NOx, g/mi | PM, mg/mi | |
|-----------|---|------------|----------------|-----------|-----------|
| Vehicle A | EPA Tier 3 Bin 125 Certification Standard | 2.1 | 0.125 | 3 | |
| | FTP-75 Checkout Results | 0.26 | 0.029 | 0.7 | |
| | | | | | |
| Vehicle C | EPA Tier 3 Bin 30 Certification Standard | 1 | 0.03 | 3 | |
| | FTP-75 Checkout Results | 0.334 | 0.005 | 0.6 | |
| | | | | | |
| Vehicle D | EPA Tier 3 Bin 30 Certification Standard | 1 | 0.03 | 3 | |
| | FTP-75 Checkout Results | 0.12 | 0.017 | 0.6 | |
| | | | | | |
| | | NMOG, g/mi | CO, g/mi | NOx, g/mi | PM, mg/mi |
| Vehicle B | EPA Tier 2 Bin 5 Certification Standard | 0.09 | 4.2 | 0.07 | 10 |
| | FTP-75 Checkout Results | 0.027 | 0.195 | 0.024 | 4.9 |

3.2.2 Test Vehicle Issues

Several problems were encountered with individual vehicles early in the program. All problems were overcome, and void tests were repeated when necessary. This section describes each problem and the resulting solution.

During the first test set, Vehicle D did not operate correctly in hybrid vehicle mode (HV) as originally planned. Instrumentation installed to measure tractive battery voltage triggered a fault code and forced the vehicle to operate in charge depleting mode (EV) rather than HV. Those tests were repeated during the second interval with that particular fuel (Fuel B). Additionally, Vehicle D experienced an HEV fault during one of the LA92 tests and could not complete the cycle. This test was also repeated.

Vehicle C's engine start/stop feature did not function properly for the first set of tests. The team investigated and found that start/stop would not operate correctly when driven on a two-wheel drive chassis dynamometer. SwRI installed circuitry to measure the wheel speed from the front wheels and emulate the measured speed to the ECU, in place of the rear wheel speed sensors. This temporarily allowed start/stop to function correctly; however, start/stop would revert to being inoperable after one or two tests on the dynamometer. This problem was remedied by using OEM software to initiate vehicle rolls mode. This allows for start/stop to operate correctly on the dynamometer. Tests conducted with start/stop inoperable were rerun.

3.3 Test Cycle

A 3-Phase cold-start LA92 drive schedule was used for all tests in this project. Figure 2 shows the first two phases of this schedule. The LA92 is run in the following manner: Phase 1

and Phase 2 are run consecutively, followed by a ten-minute hot soak, then Phase 3 is run, which is a duplicate of Phase 1. Only Phase 1 particulate emissions data was measured and used for the PMI model validation, however, gaseous emissions from all three phases were measured.

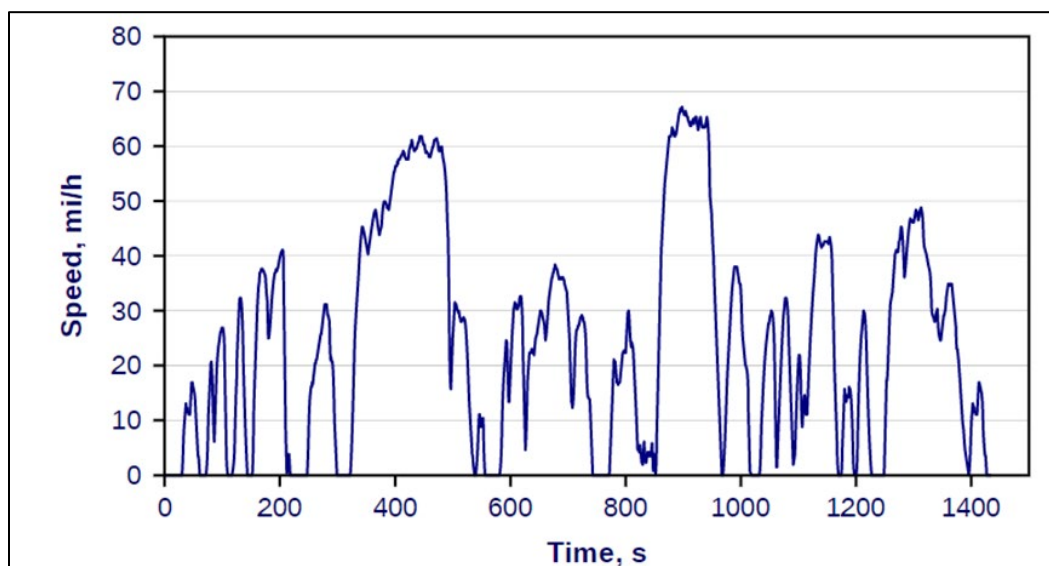


FIGURE 3. PHASE 1 AND 2 OF THE LA92 DRIVE CYCLE

3.4 Chassis Dynamometer

Emissions testing was conducted on a Horiba 48-inch single-roll chassis dynamometer. The dynamometer can electrically simulate inertia weights up to 15,000 lb over the FTP-75, and provide programmable road-load simulation of up to 200 hp continuous at 65 mph. SwRI derived set road load coefficients using inertia settings and target road-load coefficients from the EPA database for each test vehicle. Table 4 gives the target and derived set road-load coefficients for each vehicle. The same chassis dynamometer and driver were used for all testing in this project. During the soak periods, conventional vehicles were fitted with a trickle charger to maintain battery condition. Vehicle D (hybrid) was connected to a level two charger during soak periods.

TABLE 4. CHASSIS DYNAMOMETER LOAD SETTINGS

| Vehicle ID | A | B | C | D |
|----------------|---------|----------|---------|----------|
| Target | | | | |
| ETW (lbs) | 4750 | 4000 | 4750 | 3625 |
| A (lbf) | 26.79 | 26.347 | 38.24 | 18.816 |
| B (lbf/mph) | 0.6021 | 0.40519 | 0.2803 | 0.38689 |
| C (lbf/mph**2) | 0.0166 | 0.021578 | 0.02328 | 0.012501 |
| Set | | | | |
| ETW (lbs) | 4750 | 4000 | 4750 | 3625 |
| A (lbf) | 11.62 | 9.67 | 19.81 | 9.79 |
| B (lbf/mph) | 0.0765 | 0.079 | 0.1647 | -0.0465 |
| C (lbf/mph**2) | 0.01998 | 0.02195 | 0.02167 | 0.01684 |

3.5 Laboratory Emissions Sampling Systems

For determination of exhaust emissions and fuel economy by the carbon balance method, bagged exhaust emission concentrations of THC, CO, methane (CH₄) (for determination of NMHC), NO_x, and CO₂ were determined in a manner consistent with light-duty vehicle testing protocols given in 40 CFR Part 1066. A Horiba Constant Volume Sampler (CVS) was used to collect dilute exhaust in Kynar bags. For the determination of PM emissions, a proportional sample of dilute exhaust was drawn through a 47mm Whatman Teflon membrane filter following Part 1066 protocols. PM was measured for Phase 1 of the LA92 cycle only. Gaseous measurements were taken for all phases. Partway through the project, in January 2021, measurement of exhaust soot was added as a cross check for PM. Soot was measured from dilute exhaust using an AVL Micro Soot Sensor (MSS). The pollutants were analyzed as follows:

| <u>Constituent</u> | <u>Analysis Method</u> |
|-----------------------|----------------------------------|
| Total Hydrocarbon | Flame Ionization Detector |
| Methane | Gas Chromatograph |
| Carbon Monoxide | Non-Dispersive Infrared Detector |
| Carbon Dioxide | Non-Dispersive Infrared Detector |
| Oxides of Nitrogen | Chemiluminescent Detector |
| Particulate Mass | Gravimetric Measurement |
| Soot (added Jan 2021) | AVL Micro Soot Sensor |

Figure 3 shows the test cell layout for this project.

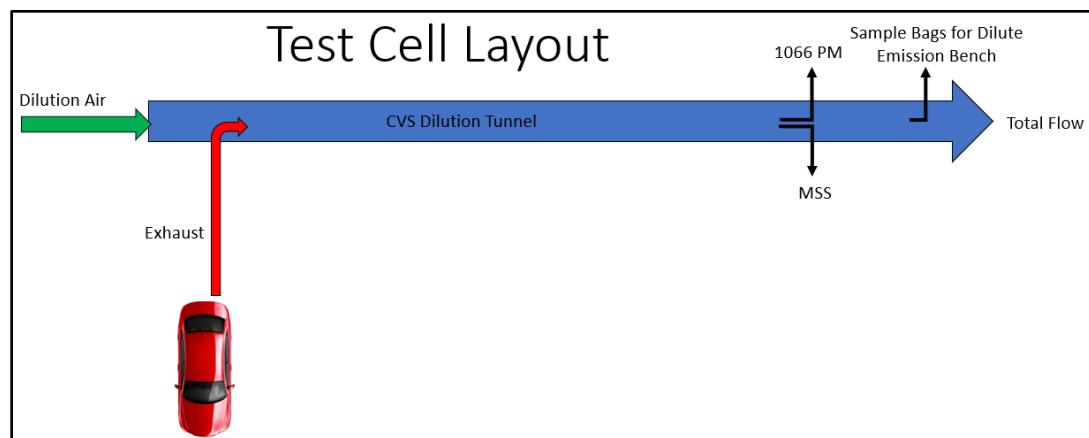


FIGURE 4. TEST CELL LAYOUT

3.6 On-Board Diagnostic (OBD)

On-board Diagnostic (OBD) data was recorded throughout each test. Below is a list of recorded OBD channels. Not all channels were available for each vehicle.

- Engine coolant temperature
- Fuel flow rate
- Engine speed
- Intake air temperature
- Mass air flow rate
- Fuel rail pressure
- Barometric pressure
- Ambient air temperature
- Engine oil temperature
- Engine fuel rate
- Lambda
- Engine load
- Torque
- Accelerator pedal position
- Fuel rail pressure

3.7 Test Procedure and Experimental Design

This project was conducted in parallel with E-122-2 and E-133 when a common fuel was tested. Those projects were originally scheduled to run a single LA92 cycle as one of the preconditioning steps during a fuel change sequence. RW-107-3 added the previously discussed emission measurements to the original LA92 cycle along with one or two additional LA92 cycles, depending on repeatability of the first two tests. The repeatability criteria was 30% for THC and 50% for both CO and NO_x. If any of these criteria failed, then the vehicle was tested a third time. Each fuel was tested using the steps below. Steps 9 through 13 indicate tasks added by RW-107-3, when run in parallel with E-122-2 or E-133. When a fuel unique to RW-107-3 was tested, all steps were conducted under this project.

Test Procedure Steps:

-
- 1. Conduct a fuel drain/fill using test fuel
 - 2. Conduct a sulfur purge
 - 3. Conduct vehicle coast downs
 - 4. Conduct a 2nd and 3rd drain/fill using test fuel
 - 5. Soak vehicle for 12 hours
 - 6. Conduct prep cycles (UDDS + HwFET + US06)
 - 7. Soak vehicle for 12 hours
 - 8. Conduct 1st cold-start LA92 with gaseous and PM emission measurement
 - 9. Soak vehicle for 12 hours
 - 10. Conduct 2nd cold-start LA92 with gaseous and PM emission measurement
 - 11. Review data against predetermine criterion
 - 12. If required, Soak vehicle for 12 hours
 - 13. If required, Conduct a 3rd cold-start LA92 with gaseous and PM emission measurement

Details for fuel change, sulfur purge, and vehicle conditioning sequences are given in Appendix B. Each fuel-vehicle combination was tested twice or three times following steps 1-13. Because of commonalities with those projects, RW-107-3 was conducted using the same fuel-vehicle run order. Table 5 gives the run order for each vehicle and fuel combination. Steps 1-13 represent a single block in the matrix. The summer matrix began in November 2020 and was followed by the winter matrix which began in July of 2021. The fuels unique to this project were tested beginning in December 2021, with the last test conducted on January 17, 2022.

TABLE 5: VEHICLE-FUEL RUN ORDER

| Run Order | Summer Fuels Test Matrix | | | | | Winter Fuels Test Matrix | | | | | Additional Matrix | | | |
|------------|--------------------------|---|---|---|---|--------------------------|---|---|---|----|-------------------|----|----|----|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
| Vehicle ID | A | B | C | A | C | C | D | A | A | D | B | A | D | B |
| | D | C | D | D | A | A | B | D | B | C | A | C | B | A |
| | C | A | B | C | B | D | A | C | D | A | C | D | A | C |
| | B | D | A | A | D | B | C | B | C | B | D | B | C | D |

| E10 Market Fuels | |
|------------------|---------------------------|
| | Tier 3 Certification Fuel |
| | Summer E10, High PMI |
| | Summer E10, Low PMI |
| | Winter E10, High PMI |
| | Winter E10, Low PMI |

| E10 Market Fuels Blended to E15 | |
|---------------------------------|-------------------------------------|
| | Summer E10, Blended to E15 High PMI |
| | Summer E10 Blended to E15, Low PMI |
| | Winter E10 Blended to E15, High PMI |
| | Winter E10 Blended to E15, Low PMI |

| E0 Fuels and E10 & E15 Blends | |
|-------------------------------|----------------------------------|
| | Summer E0, High PMI |
| | Winter E0, Low PMI |
| | Summer E0 Blend to E10, High PMI |
| | Summer E0 Blend to E15, High PMI |

4.0 RESULTS

Figure 4 and Figure 5 show the relationship between particulate mass emissions (PM) and exhaust soot emissions (MSS) from Phase 1 of the LA92 cycle. The first figure includes all vehicles with each vehicle indicated by a different color. The PM and MSS emission rate from the Tier 2 vehicle, Vehicle B, was much higher compared to the other vehicles that were all certified to a Tier 3 standard. Linear regression lines are included for each vehicle. Vehicle B has the best linear regression fit with an R-squared value of 0.99. The other vehicles have a weaker fit, which could be caused by the lower span and range of PM and soot values. The second figure shows the same data with Vehicle B removed to improve resolution of the Tier 3 vehicle results. For all plots in this section, winter-grade, summer-grade, and certification fuels are identified with different marks styles to allow approximate identification of fuel RVP.

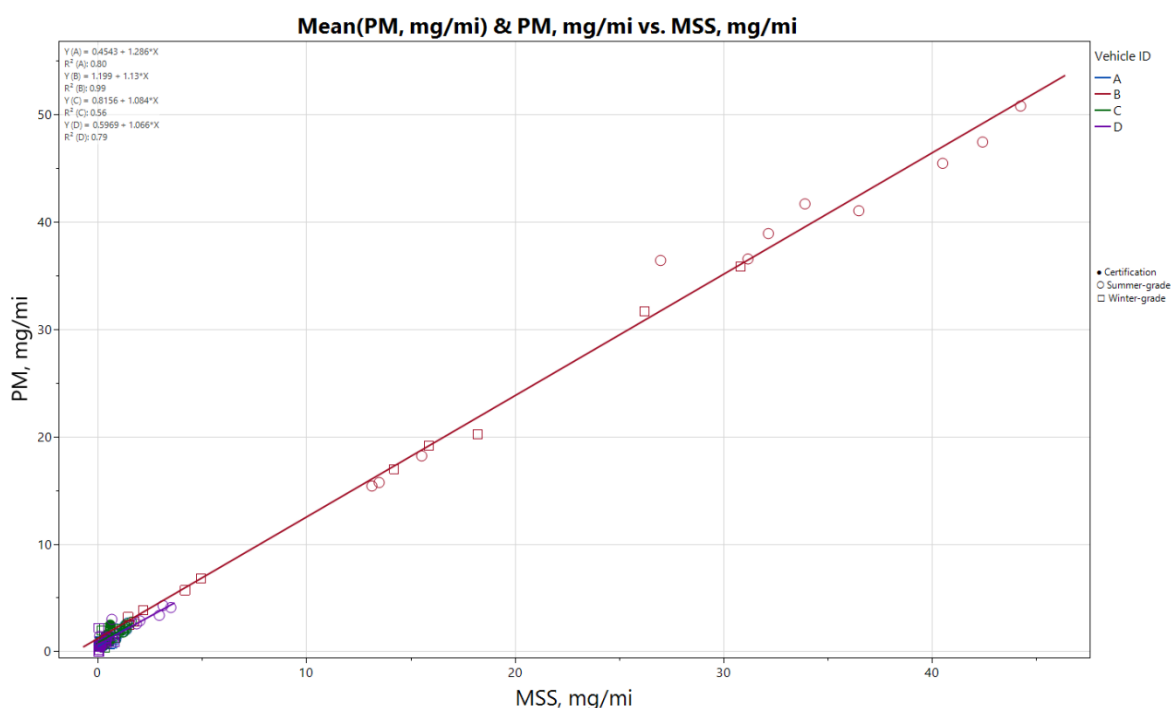


FIGURE 5. PHASE 1, MSS VS PM, ALL VEHICLES

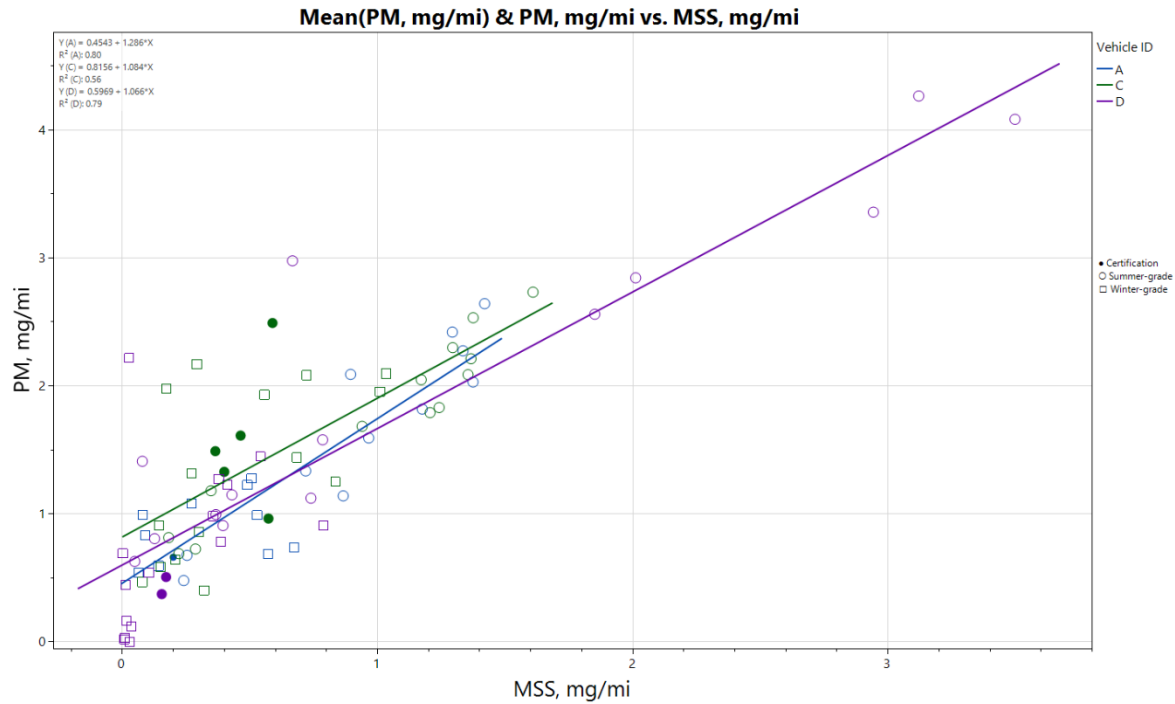


FIGURE 6. PHASE 1, MSS VS PM, WITHOUT VEHICLE B

Figure 6 through Figure 9 show either PM or MSS results from Phase 1 plotted against the test fuel PMI. A moving average line was added to indicate loose trends; however, these lines should not be used to draw robust statistical conclusions. Plots are given both with and without Vehicle B included due to the large magnitude difference previously discussed. All vehicles show an increasing trend in particulate mass and soot emissions with increasing fuel PMI, although, statistical analysis was not conducted to evaluate significance of the trend.

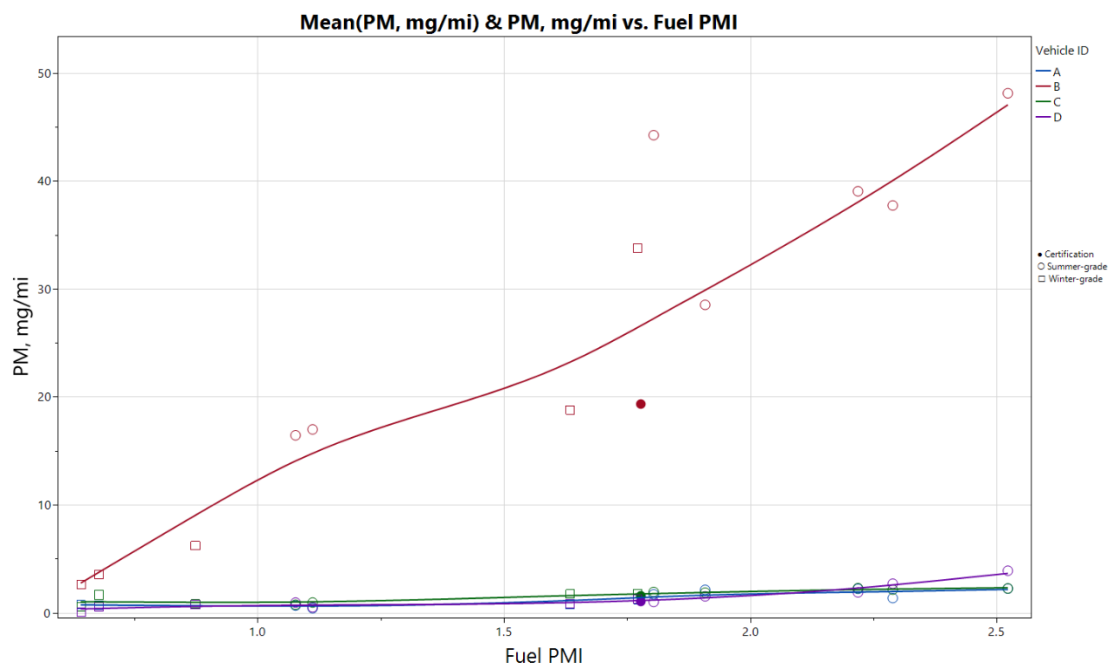


FIGURE 7. PHASE 1, FUEL PMI VS PM, ALL VEHICLES

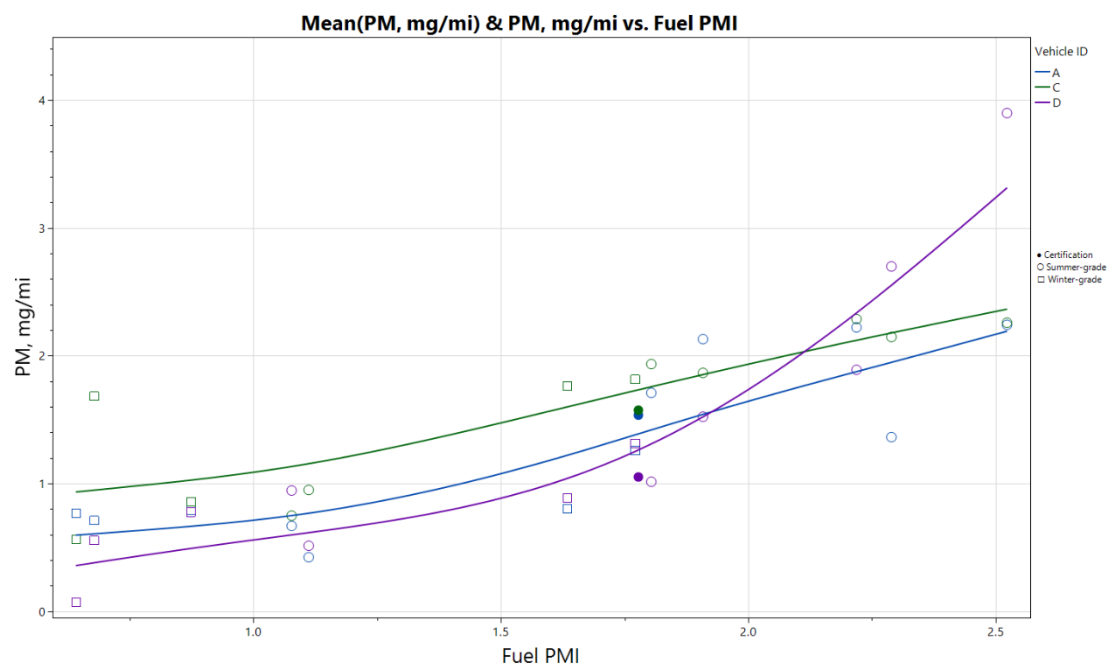


FIGURE 8. PHASE 1, FUEL PMI VS PM, WITHOUT VEHICLE B

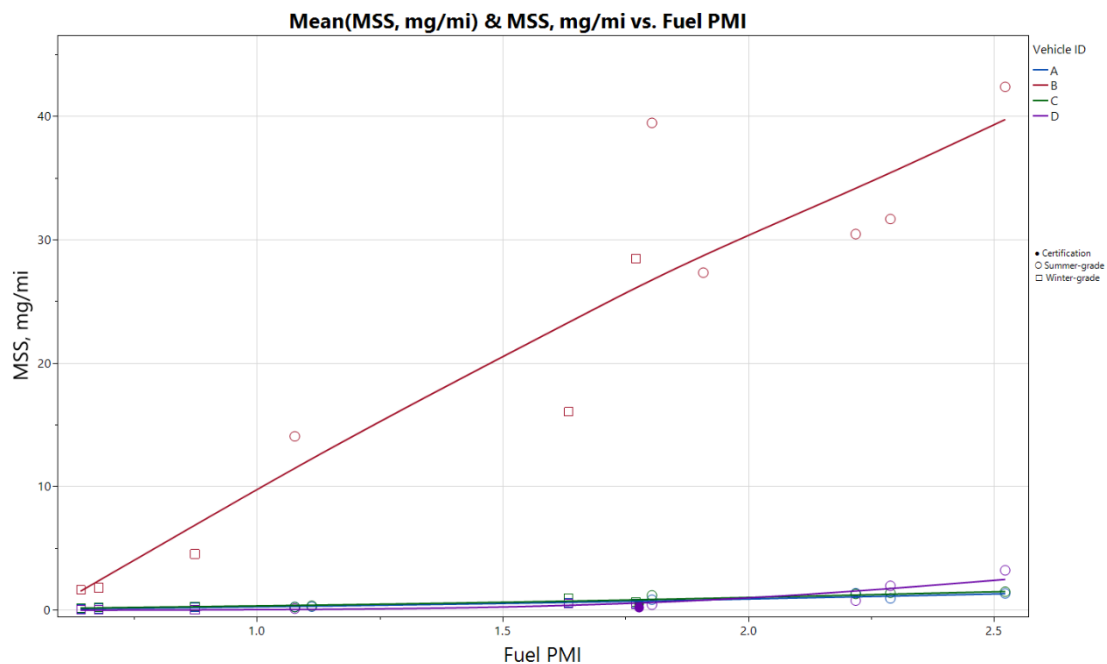


FIGURE 9. PHASE 1, FUEL PMI VS MSS, ALL VEHICLES

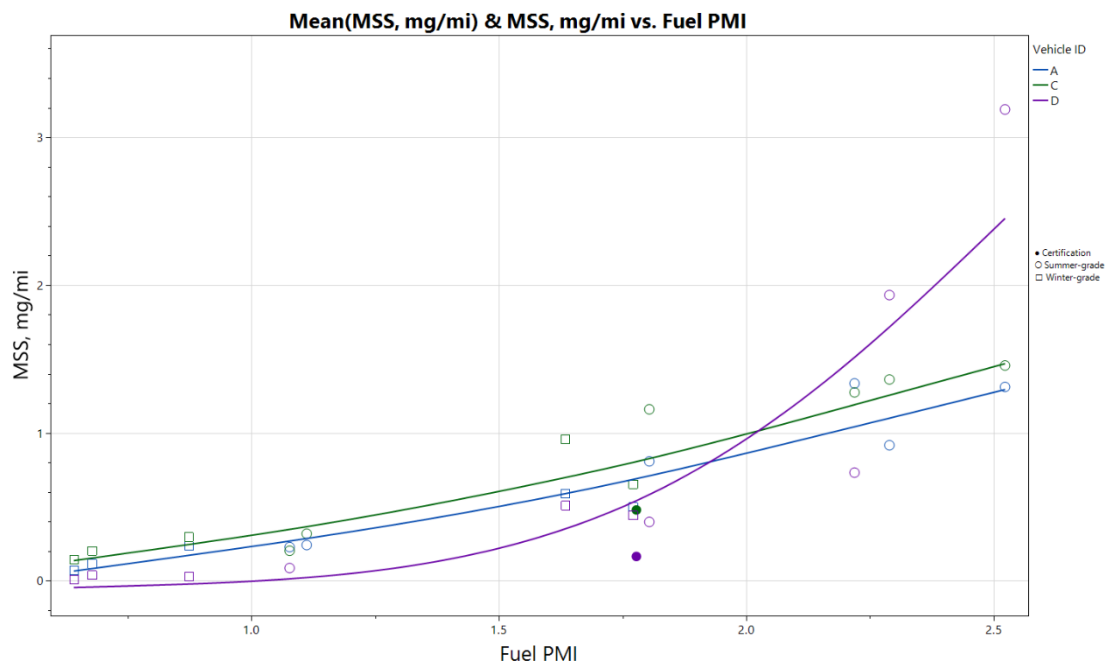


FIGURE 10. PHASE 1, FUEL PMI VS MSS, WITHOUT VEHICLE B

Figure 10 through Figure 14 give gaseous emissions from Phase 1 of the LA92 plotted against fuel PMI and Figure 15 gives the carbon balance fuel economy for this phase calculated from THC, CO, and CO₂. CO emissions appear to decrease with increasing PMI for all vehicles except Vehicle D. Fuel economy was very stable over the approximately 27-month test duration.

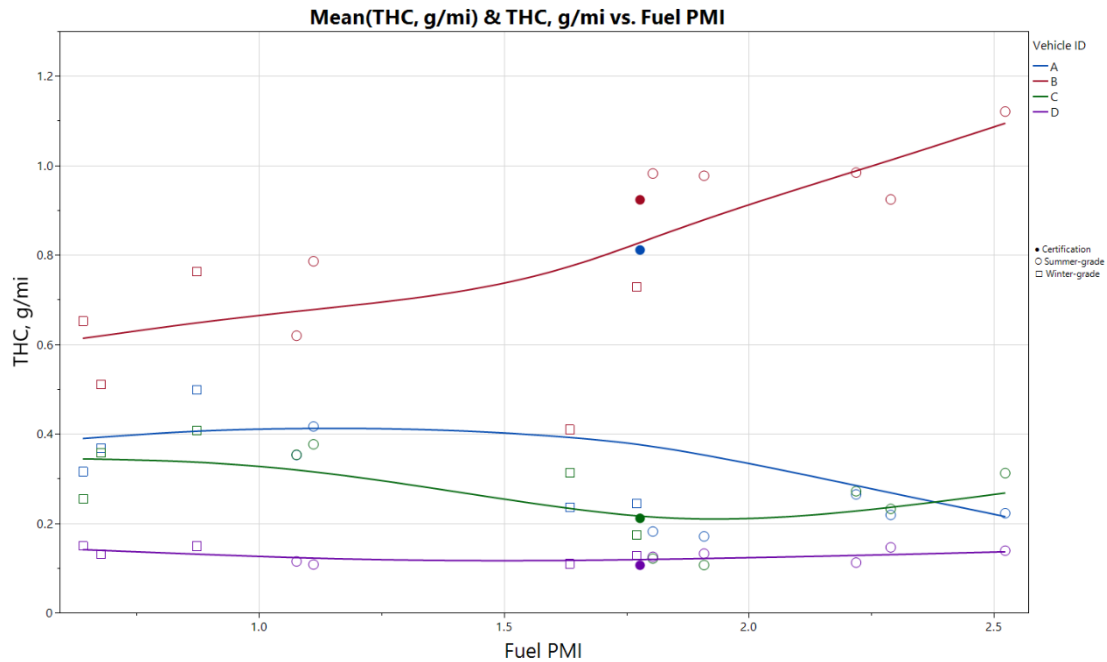


FIGURE 11. PHASE 1, FUEL PMI VS THC, ALL VEHICLES

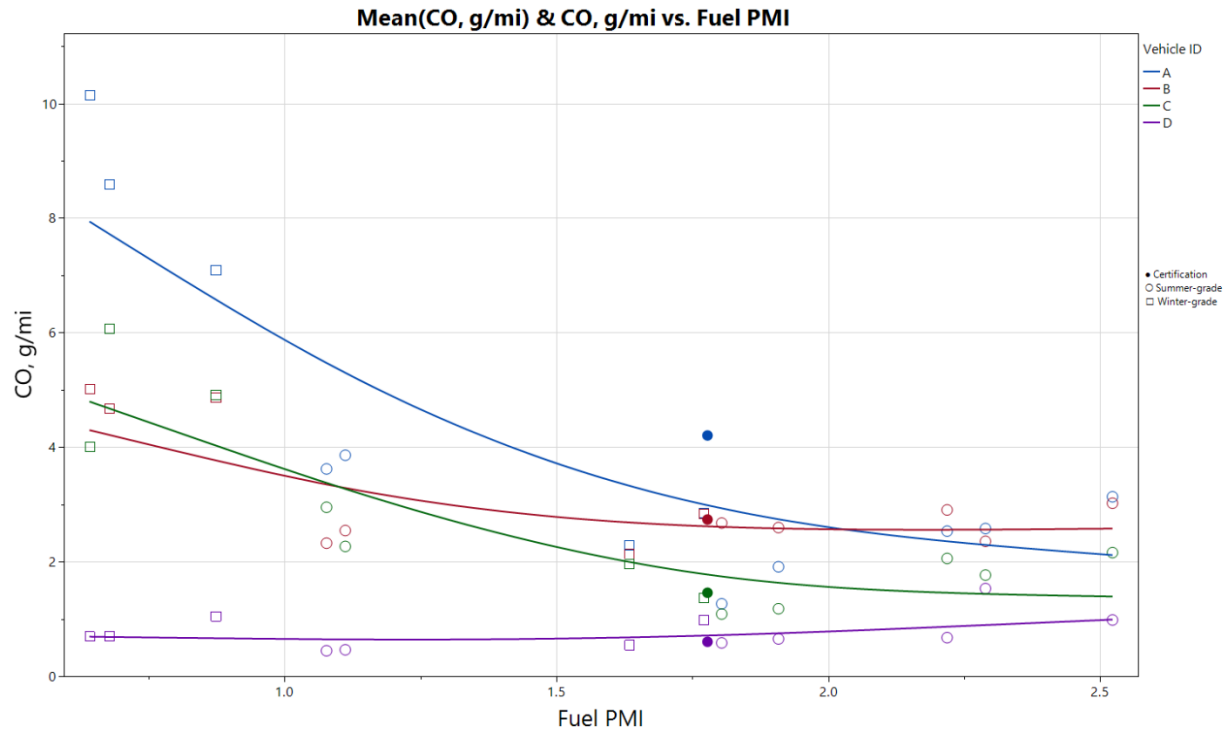


FIGURE 12. PHASE 1, FUEL PMI VS CO, ALL VEHICLES

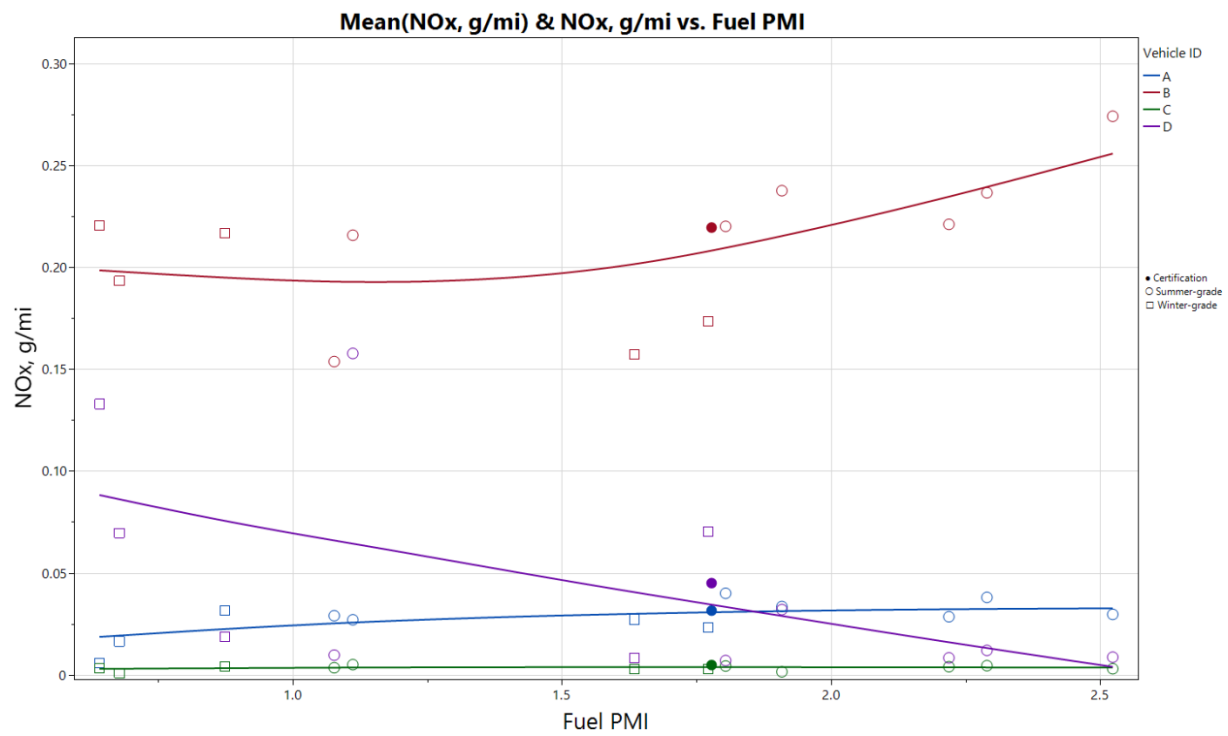


FIGURE 13. PHASE 1, FUEL PMI VS NOx, ALL VEHICLES

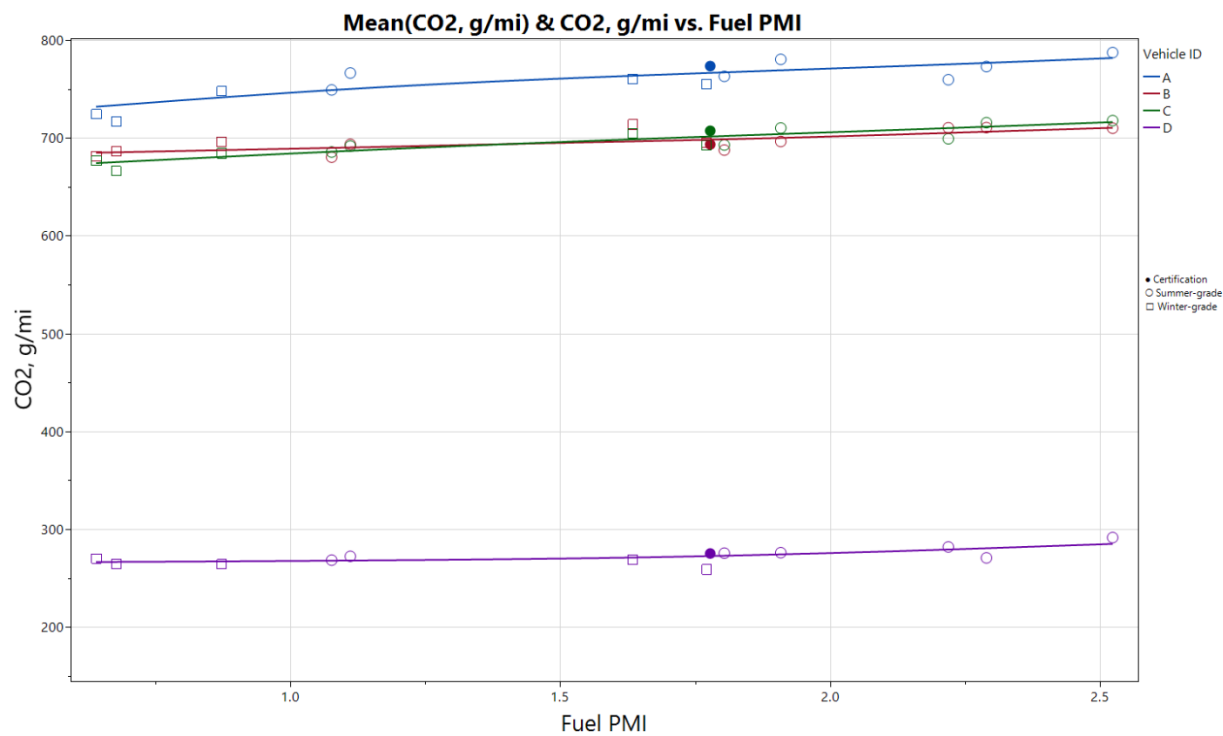


FIGURE 14. PHASE 1, FUEL PMI VS CO₂, ALL VEHICLES

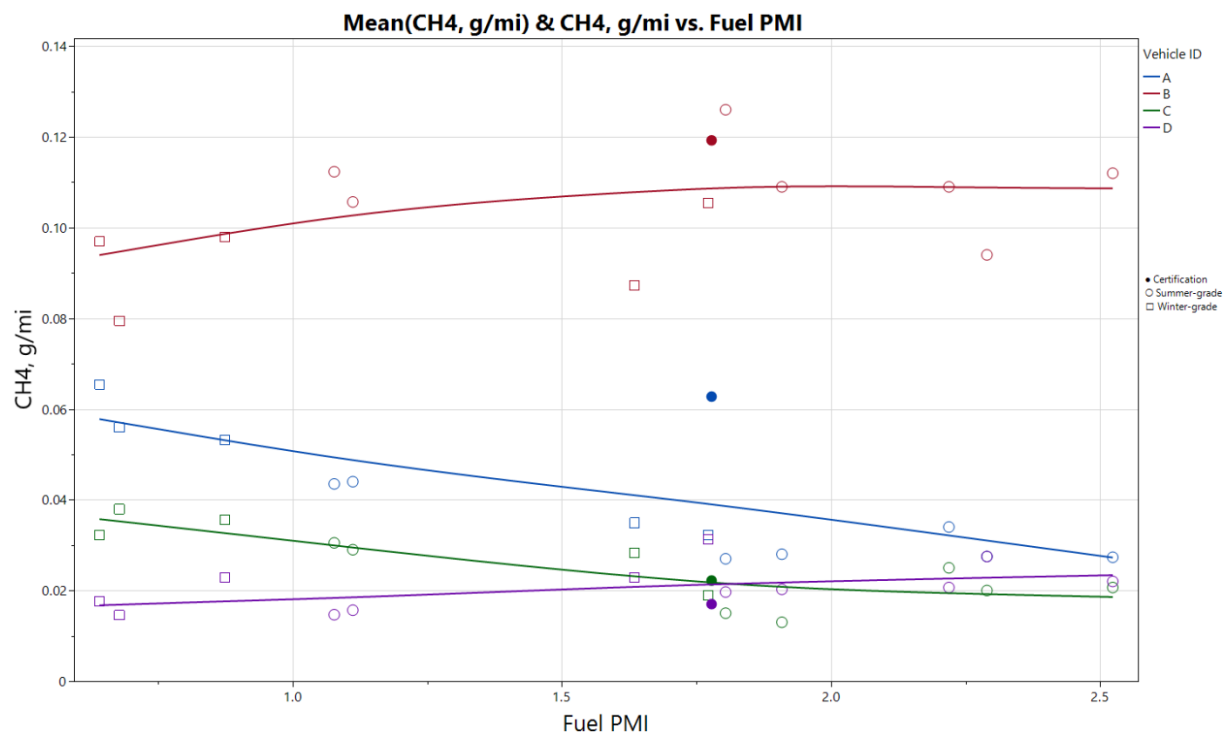


FIGURE 15. PHASE 1, FUEL PMI VS CH₄, ALL VEHICLES

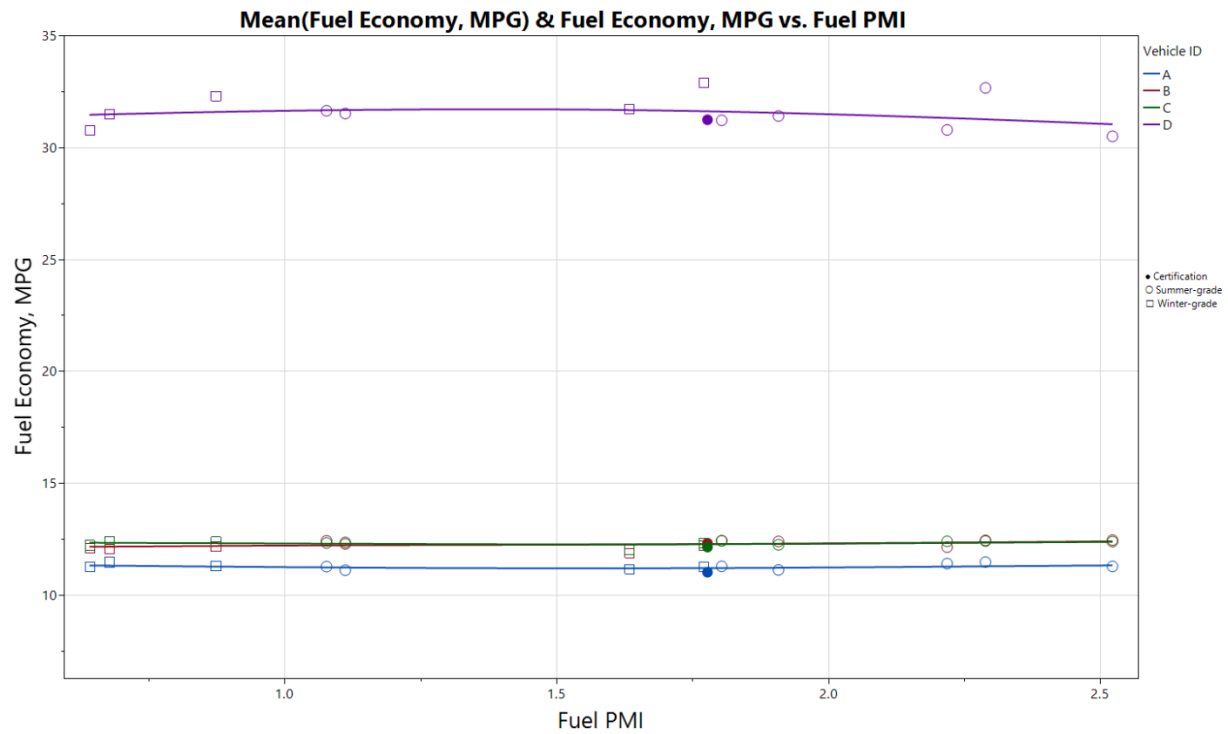


FIGURE 16. PHASE 1, FUEL PMI VS FUEL ECONOMY, ALL VEHICLES

Results from all valid tests are given in table form in Appendix C. This table provides phases 1, 2, 3, and the total LA92 result separately. As previously discussed, statistical analysis of the results was conducted by a separate contractor and conclusions from that analysis are reported separately from this document.

APPENDIX A

TEST FUEL ACQUISITION AND ANALYSES

Appendix A. Test Fuel Acquisition and Analyses

Six commercial test fuels were obtained by SwRI for this program. The fuels were differentiated by a winter batch and a summer batch. Both high and low PMI fuels were obtained for each batch. SwRI acquired these fuels with the help of CRC members who identified locations based on internal analyses. For the first four E10 fuels CRC initially targeted 1,700 gallons of each fuel but then increased this volume to 2,200 gallons. For the summer E0 batch CRC requested that 650 gallons be purchased and for the winter E0 batch only 200 gallons was requested by CRC to be purchased.

Winter Fuels:

- 2,164 gallons of low PMI RUL E10 from CRC member fuel terminal
- 2,182 gallons of high PMI PUL E10 from CRC member fuel terminal
- 200 gallons of low PMI RUL E0 from CRC member fuel terminal

Summer Fuels:

- 2,152 gallons of low PMI RUL E10 from CRC member fuel terminal
- 1,686 gallons of high PMI RUL E10 from CRC member fuel terminal
- 650 gallons of high PMI E0 RUL from CRC member fuel terminal

The procedure to acquire the fuels included the following steps:

1. Steam-clean and dry a tanker truck compartment
2. Drive tanker to terminal and rinse lines and compartment with 50 gallons of desired gasoline
3. Immediately fill the rinsed compartment with the desired gasoline
4. Deliver fuel to SwRI for analysis and off-loading
5. Repeat for additional batches of fuel

Each fuel was analyzed according to the following list of analyses.

- D5191 Reid Vapor Pressure
- D4815 Oxygenates
- D5453 Sulfur
- D86 Distillation
- D381 Existent Gum
- D240 Net Heat of Combustion
- D5291 Carbon / Hydrogen
- D4052 Specific Gravity
- D2699 Research Octane Number
- D2700 Motor Octane Number
- D6729 Detailed Hydrocarbon Analyses
- D4814 Driveability Index

| | | CRC E-122-2 Fuels | | | | | |
|------------------|-------------------------------|-------------------------------------|-------------------------------|------------------------------------|-------------------------------------|--|-----------|
| | | Summer Fuels | | Winter Fuels | | | |
| | | Low PMI E10 RUL | High PMI E10 RUL | E10 Low PMI RUL | E10 High PMI PUL | | |
| Fuel Description | | Fuel B | Fuel C | Fuel D | Fuel E | | |
| CRC Fuel ID | | Marathon Terminal (Salt Lake City) | Motiva Terminal (San Antonio) | Marathon Terminal (Salt Lake City) | Chevron Richmond Technology Center | | |
| Fuel Source | | GA-10940 | GA-10920 | GA-11027 | CGA-11053 | CGB-11093 | |
| SwRI Fuel Code | | FLRD-3606 | FLRD-3560 | FLRD-3914 | FLRD-3979 | FLRD-3788 | |
| Sample Code | | FLRD-3606 | FLRD-3560 | FLRD-3914 | FLRD-3979 | FLRD-3788 | |
| Sample Source | | Drum Sample after Tanker Offloading | Tanker Manifold Sample | Tanker Manifold Sample | Drum Sample after Tanker Offloading | Sample after TOP TIER Additive Treatment | |
| Date of Sample | | 7/20/2020 | 5/29/2020 | 1/15/2021 | 3/26/2021 | 6/18/2021 | |
| Current Volume | | 2,152 gallons | 1,686 gallons | 2,164 gallons | 2,182 gallons | 2,182 gallons | |
| ASTM Method | Test Request | Test Units | Results | Results | Results | Results | Results |
| D6729 | Detailed Hydrocarbon Analysis | -- | completed | completed | completed | completed | completed |
| PMI | PM Index | calculated | 1.1115 | 1.9085 | 0.6772 | 1.7708 | n/a |
| D86 | Distillation | | | | | | |
| | IBP | Deg. F | 96 | 103 | 81 | 78 | n/a |
| | 5% | Deg. F | 121 | 125 | 93 | 100 | n/a |
| | 10% | Deg. F | 130 | 131 | 103 | 109 | n/a |
| | 15% | Deg. F | 136 | 135 | 112 | 117 | n/a |
| | 20% | Deg. F | 141 | 139 | 120 | 125 | n/a |
| | 30% | Deg. F | 150 | 146 | 134 | 141 | n/a |
| | 40% | Deg. F | 158 | 153 | 146 | 155 | n/a |
| | 50% | Deg. F | 203 | 198 | 154 | 173 | n/a |
| | 60% | Deg. F | 227 | 235 | 194 | 242 | n/a |
| | 70% | Deg. F | 246 | 264 | 224 | 268 | n/a |
| | 80% | Deg. F | 273 | 297 | 248 | 302 | n/a |
| | 90% | Deg. F | 306 | 330 | 281 | 338 | n/a |
| | 95% | Deg. F | 333 | 351 | 303 | 367 | n/a |
| | FBP | Deg. F | 367 | 403 | 344 | 392 | n/a |
| | Recovered | mL | 98 | 98.4 | 97 | 97 | n/a |
| | Residue | mL | 0.9 | 0.7 | 0.7 | 0.7 | n/a |
| | Loss | mL | 1.6 | 0.9 | 2.2 | 2.0 | n/a |
| D86 | Driveability Index | -- | 1109.8 | 1119.5 | 896.7 | 971.2 | n/a |
| D5191 | Vapor Pressure (Mini Method) | | | | | | |
| | RVP (EPA Equation) | psi | 8.98 | 7.73 | 15.25 | 13.64 | n/a |
| | DVPE (ASTM Equation) | psi | 8.87 | 7.61 | 15.2 | 13.57 | n/a |
| D240 | Heat of Combustion | | | | | | |
| | GROSS | BTU/lb | 19244 | 19147 | 19494 | 19225 | n/a |
| | GROSS | MJ/kg | 44.760 | 44.536 | 45.344 | 44.717 | n/a |
| | GROSS | cal/g | 10690.8 | 10637.2 | 10830.3 | 10680.6 | n/a |
| D240 | Heat of Combustion | | | | | | |
| | NET | BTU/lb | 17982 | 17917 | 18204 | 17968 | n/a |
| | NET | MJ/kg | 41.827 | 41.675 | 42.941 | 41.794 | n/a |
| | NET | cal/g | 9990.3 | 9953.9 | 10113.1 | 9982.2 | n/a |
| D2699 | Research Octane Number (RON) | -- | 92.5 | 91.2 | 91 | 97.2 | n/a |
| D2700 | Motor Octane Number (MON) | -- | 83.7 | 82.7 | 82.9 | 87.9 | n/a |
| D381 | Existent Gums Content | | | | | | |
| | Unwashed Wt | mg/100 mL | 9.5 | 16.0 | 9.5 | 1.5 | 20.0 |
| | Washed Wt | mg/100 mL | <0.5 | <0.5 | <0.5 | 0.5 | 0.5 |
| D4052 | API Gravity | -- | 60.1 | 57.5 | 66.1 | 60.7 | n/a |
| | Specific Gravity | -- | 0.7386 | 0.7486 | 0.7161 | 0.7362 | n/a |
| | Density @ 15°C | g/mL | 0.7384 | 0.7484 | 0.7160 | 0.7360 | n/a |
| D4815 | Oxygenates and Oxygen Content | | | | | | |
| | Methanol (MeOH) | vol% | <0.3 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethanol (EtOH) | vol% | 9.71 | 9.50 | 9.55 | 10.19 | n/a |
| | Isopropanol (iPA) | vol% | <0.2 | <0.2 | 10.58 | <0.2 | n/a |
| | tert-Butanol (tBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | n-Propanol (nPA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Methyl tert-butylether (MTBE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | sec-Butanol (sBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Diisopropylether (DIPE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Isobutanol (iBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethyl tert-butylether (ETBE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | tert-Pentanol (tPA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | n-Butanol (nBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | tert-amyl methylether (TAME) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethanol (EtOH) | wt% | 10.43 | 10.07 | <0.2 | 10.99 | n/a |
| | Total Oxygen | wt% | 3.62 | 3.49 | 3.67 | 3.81 | n/a |
| D5291 | Carbon Content | wt% | 82.32 | 83.12 | 82.30 | 82.33 | n/a |
| | Hydrogen Content | wt% | 13.83 | 13.48 | 14.15 | 13.78 | n/a |
| D5453 | Sulfur by UV | ppm | 7.1 | 6.2 | 11.4 | 5.1 | n/a |

| | | CRC E-122-2 Fuels | | | | | |
|------------------|-------------------------------|-------------------------------------|-------------------------------|------------------------------------|-------------------------------------|--|-----------|
| | | Summer Fuels | | Winter Fuels | | | |
| | | Low PMI E10 RUL | High PMI E10 RUL | E10 Low PMI RUL | E10 High PMI PUL | | |
| Fuel Description | | Fuel B | Fuel C | Fuel D | Fuel E | | |
| CRC Fuel ID | | Marathon Terminal (Salt Lake City) | Motiva Terminal (San Antonio) | Marathon Terminal (Salt Lake City) | Chevron Richmond Technology Center | | |
| Fuel Source | | GA-10940 | GA-10920 | GA-11027 | CGA-11053 | CGB-11093 | |
| SwRI Fuel Code | | FLRD-3606 | FLRD-3560 | FLRD-3914 | FLRD-3979 | FLRD-3788 | |
| Sample Code | | FLRD-3606 | FLRD-3560 | FLRD-3914 | FLRD-3979 | FLRD-3788 | |
| Sample Source | | Drum Sample after Tanker Offloading | Tanker Manifold Sample | Tanker Manifold Sample | Drum Sample after Tanker Offloading | Sample after TOP TIER Additive Treatment | |
| Date of Sample | | 7/20/2020 | 5/29/2020 | 1/15/2021 | 3/26/2021 | 6/18/2021 | |
| Current Volume | | 2,152 gallons | 1,686 gallons | 2,164 gallons | 2,182 gallons | 2,182 gallons | |
| ASTM Method | Test Request | Test Units | Results | Results | Results | Results | Results |
| D6729 | Detailed Hydrocarbon Analysis | -- | completed | completed | completed | completed | completed |
| PMI | PM Index | calculated | 1.1115 | 1.9085 | 0.6772 | 1.7708 | n/a |
| D86 | Distillation | | | | | | |
| | IBP | Deg. F | 96 | 103 | 81 | 78 | n/a |
| | 5% | Deg. F | 121 | 125 | 93 | 100 | n/a |
| | 10% | Deg. F | 130 | 131 | 103 | 109 | n/a |
| | 15% | Deg. F | 136 | 135 | 112 | 117 | n/a |
| | 20% | Deg. F | 141 | 139 | 120 | 125 | n/a |
| | 30% | Deg. F | 150 | 146 | 134 | 141 | n/a |
| | 40% | Deg. F | 158 | 153 | 146 | 155 | n/a |
| | 50% | Deg. F | 203 | 198 | 154 | 173 | n/a |
| | 60% | Deg. F | 227 | 235 | 194 | 242 | n/a |
| | 70% | Deg. F | 246 | 264 | 224 | 268 | n/a |
| | 80% | Deg. F | 273 | 297 | 248 | 302 | n/a |
| | 90% | Deg. F | 306 | 330 | 281 | 338 | n/a |
| | 95% | Deg. F | 333 | 351 | 303 | 367 | n/a |
| | FBP | Deg. F | 367 | 403 | 344 | 392 | n/a |
| | Recovered | mL | 98 | 98.4 | 97 | 97 | n/a |
| | Residue | mL | 0.9 | 0.7 | 0.7 | 0.7 | n/a |
| | Loss | mL | 1.6 | 0.9 | 2.2 | 2.0 | n/a |
| D86 | Driveability Index | -- | 1109.8 | 1119.5 | 896.7 | 971.2 | n/a |
| D5191 | Vapor Pressure (Mini Method) | | | | | | |
| | RVP (EPA Equation) | psi | 8.98 | 7.73 | 15.25 | 13.64 | n/a |
| | DVPE (ASTM Equation) | psi | 8.87 | 7.61 | 15.2 | 13.57 | n/a |
| D240 | Heat of Combustion | | | | | | |
| | GROSS | BTU/lb | 19244 | 19147 | 19494 | 19225 | n/a |
| | GROSS | MJ/kg | 44.760 | 44.536 | 45.344 | 44.717 | n/a |
| | GROSS | cal/g | 10690.8 | 10637.2 | 10830.3 | 10680.6 | n/a |
| D240 | Heat of Combustion | | | | | | |
| | NET | BTU/lb | 17982 | 17917 | 18204 | 17968 | n/a |
| | NET | MJ/kg | 41.827 | 41.675 | 42.941 | 41.794 | n/a |
| | NET | cal/g | 9990.3 | 9953.9 | 10113.1 | 9982.2 | n/a |
| D2699 | Research Octane Number (RON) | -- | 92.5 | 91.2 | 91 | 97.2 | n/a |
| D2700 | Motor Octane Number (MON) | -- | 83.7 | 82.7 | 82.9 | 87.9 | n/a |
| D381 | Existent Gums Content | | | | | | |
| | Unwashed Wt | mg/100 mL | 9.5 | 16.0 | 9.5 | 1.5 | 20.0 |
| | Washed Wt | mg/100 mL | <0.5 | <0.5 | <0.5 | 0.5 | 0.5 |
| D4052 | API Gravity | -- | 60.1 | 57.5 | 66.1 | 60.7 | n/a |
| | Specific Gravity | -- | 0.7386 | 0.7486 | 0.7161 | 0.7362 | n/a |
| | Density @ 15°C | g/mL | 0.7384 | 0.7484 | 0.7160 | 0.7360 | n/a |
| D4815 | Oxygenates and Oxygen Content | | | | | | |
| | Methanol (MeOH) | vol% | <0.3 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethanol (EtOH) | vol% | 9.71 | 9.50 | 9.55 | 10.19 | n/a |
| | Isopropanol (iPA) | vol% | <0.2 | <0.2 | 10.58 | <0.2 | n/a |
| | tert-Butanol (tBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | n-Propanol (nPA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Methyl tert-butylether (MTBE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | sec-Butanol (sBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Diisopropylether (DIPE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Isobutanol (iBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethyl tert-butylether (ETBE) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | tert-Pentanol (tPA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | n-Butanol (nBA) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | tert-amyl methylether (TAME) | vol% | <0.2 | <0.2 | <0.2 | <0.2 | n/a |
| | Ethanol (EtOH) | wt% | 10.43 | 10.07 | <0.2 | 10.99 | n/a |
| | Total Oxygen | wt% | 3.62 | 3.49 | 3.67 | 3.81 | n/a |
| D5291 | Carbon Content | wt% | 82.32 | 83.12 | 82.30 | 82.33 | n/a |
| | Hydrogen Content | wt% | 13.83 | 13.48 | 14.15 | 13.78 | n/a |
| D5453 | Sulfur by UV | ppm | 7.1 | 6.2 | 11.4 | 5.1 | n/a |

| | | CRC E-133 Fuels | | | | |
|-------------------|--------------------------------|--------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| | | Summer Fuels | | Winter Fuels | | |
| | | Fuel Description | Low PMI E15 | High PMI E15 | Low PMI E15 | High PMI E15 |
| | | Fuel Name | Fuel F (splash blend of Fuel B) | Fuel G (splash blend of Fuel C) | Fuel H (splash blend of Fuel D) | Fuel I (splash blend of Fuel E) |
| | | SwRI Fuel Code | CGB-11037 | CGB-11039 | CGB-11156 | CGB-11149 |
| Fuel Blend Number | 2021-005 | 2021-006 | 2021-031 | 2021-032 | | |
| Sample Location | Tote 08-0305 | Tote 08-0375 | Tote 08-038s | Tote 08-030s | | |
| Sample Code | FLRD-3938/FLRD-3945/FLRD-4250 | FLRD-3939/FLRD-3946/FLRD-4251 | FLRD-4209 / FLRD-4213 | FLRD-4190 / FLRD-4199 | | |
| Sample Dates | 3/1/2021 - 3/5/2021 - 11/02/21 | 3/3/2021 - 3/5/2021 - 11/02/21 | 9/27/01 & 9/20/2021 | 9/7/2021 & 9/20/2021 | | |
| ASTM Method | Test Request | Test Units | Results | Results | Results | |
| D5191 | Vapor Pressure (Mini Method) | | | | | |
| | RVP (EPA Equation) | psi | 8.74 | 7.58 | 14.21 | 13.3 |
| | DVPE (ASTM Equation) | psi | 8.63 | 7.45 | 14.15 | 13.22 |
| D4052 | API Gravity | -- | 59.2 | 56.8 | 63.2 | 59.8 |
| | Specific Gravity | -- | 0.7419 | 0.7514 | 0.7268 | 0.7396 |
| | Density @ 15°C | g/mL | 0.7417 | 0.7511 | 0.7265 | 0.7393 |
| | Density @ 15°C | g/L | 741.7 | 751.1 | 726.5 | 739.3 |
| D5599 | Oxygenates and Oxygen Content | | | | | |
| | Diisopropylether (DIPE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Ethyl tert-butylether (ETBE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Ethanol (EtOH) | vol% | 15.23 | 14.95 | 15.31 | 15.27 |
| | Ethanol (EtOH) | WT% | 16.30 | 15.80 | 16.83 | 16.39 |
| | Isobutanol (iBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Isopropanol (iPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Methanol (MeOH) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Methyl tert-butylether (MTBE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | n-Butanol (nBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | n-Propanol (nPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | sec-Butanol (sBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-amyl methylether (TAME) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-Butanol (tBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-Pentanol (tPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Total Oxygen | WT% | 5.66 | 5.48 | 5.84 | 5.69 |
| D5599 | Oxygenates and Oxygen Content | | | | | |
| duplicate | Diisopropylether (DIPE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Ethyl tert-butylether (ETBE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Ethanol (EtOH) | vol% | 14.81 | 15.09 | 15.14 | 15.31 |
| | Ethanol (EtOH) | WT% | 15.85 | 15.94 | 16.53 | 16.39 |
| | Isobutanol (iBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Isopropanol (iPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Methanol (MeOH) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Methyl tert-butylether (MTBE) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | n-Butanol (nBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | n-Propanol (nPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | sec-Butanol (sBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-amyl methylether (TAME) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-Butanol (tBA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | tert-Pentanol (tPA) | vol% | <0.1 | <0.1 | <0.1 | <0.1 |
| | Total Oxygen | WT% | 5.5 | 5.53 | 5.74 | 5.69 |
| D240 | Heat of Combustion | | | | | |
| | GROSS | BTU/lb | 18870 | 18720 | 18989 | 18736 |
| | GROSS | MI/kg | 43.89 | 43.543 | 44.168 | 43.579 |
| | GROSS | cal/g | 10483 | 10400 | 10549.4 | 10408.6 |
| D240 | Heat of Combustion | | | | | |
| | NET | BTU/lb | 17596 | 17492 | 17705 | 17484 |
| | NET | MI/kg | 40.929 | 40.685 | 41.182 | 40.667 |
| | NET | cal/g | 9775.8 | 9717.5 | 9836.1 | 9713.1 |
| D2622 | Sulfur by X-ray | ppm | 8.5 | 8.0 | 10.9 | 5.3 |
| D2699 | Research Octane Number (RON) | -- | 94.3 | 93.8 | 94.7 | 99.7 |
| D2700 | Motor Octane Number (MON) | -- | 84.7 | 84.4 | 84 | 88.7 |
| D5291 | Carbon Content | wt% | 80.66 | 80.58 | 79.88 | 80.61 |
| | Hydrogen Content | wt% | 13.95 | 13.46 | 14.08 | 13.72 |
| D6729 | DHA Analysis | -- | Complete | Complete | Complete | Complete |
| PMI | Particulate Matter Index | -- | 1.0769 | 1.8040 | 0.6408 | 1.6348 |
| D86 | Distillation | | | | | |
| | IBP | Deg. F | 95 | 101 | 80 | 80 |
| | 5% | Deg. F | 123 | 126 | 94 | 99 |
| | 10% | Deg. F | 132 | 133 | 106 | 109 |
| | 15% | Deg. F | 139 | 137 | 115 | 117 |
| | 20% | Deg. F | 144 | 141 | 123 | 125 |
| | 30% | Deg. F | 152 | 149 | 138 | 142 |
| | 40% | Deg. F | 157 | 156 | 149 | 156 |
| | 50% | Deg. F | 161 | 161 | 156 | 164 |
| | 60% | Deg. F | 217 | 213 | 161 | 195 |
| | 70% | Deg. F | 242 | 256 | 215 | 261 |
| | 80% | Deg. F | 269 | 290 | 245 | 292 |
| | 90% | Deg. F | 305 | 325 | 280 | 329 |
| | 95% | Deg. F | 330 | 348 | 306 | 352 |
| | FBP | Deg. F | 373 | 395 | 344 | 396 |
| | Recovered | mL | 98.4 | 98.3 | 96.3 | 97.8 |
| | Residue | mL | 0.7 | 0.8 | 0.9 | 1.0 |
| | Loss | mL | 0.9 | 0.9 | 2.8 | 1.2 |
| D86 | Driveability Index | -- | 987.2 | 1007.3 | 905.9 | 985.2 |

| | | CRC RW-107-3 Fuels | | | |
|------------------|-------------------------------|---------------------------------|--------------------------|--------------------------|------------------------------------|
| | | Summer Fuels | | | Winter Fuel |
| | | High PMI E0 RUL | High PMI E10 RUL | High PMI E15 RUL | Low PMI E0 RUL |
| Fuel Description | | Fuel J | Fuel L | Fuel M | Fuel K |
| CRC Fuel ID | | Phillips 66 Terminal (Westlake) | Fuel J, Splash-Blend E10 | Fuel J, Splash-Blend E15 | Marathon Terminal (Salt Lake City) |
| SwRI Fuel Code | | GA-10950 | CGB-11147 | CGB-11148 | GA-11026 |
| Sample Code | | FLRD-3627 | FLRD-4191, FLRD-4200 | FLRD-4192, FLRD-4201 | FLRD-3909 |
| Sample Source | | Tanker Manifold Sample | Tote Sample | Tote Sample | Tanker Manifold Sample |
| Date of Sample | | 7/20/2020 | 9/7/2021 / 9/20/2021 | 9/7/2021 / 9/20/2021 | 1/11/2021 |
| Current Volume | | 527 gallons | 256 gallons | 259 gallons | 195 gallons |
| ASTM Method | Test Request | Test Units | Results | Results | Results |
| D6729 | Detailed Hydrocarbon Analysis | -- | completed | completed | completed |
| PMI | PM Index | calculated | 2.5231 | 2.2894 | 2.2189 |
| D86 | Distillation | | | | |
| | IBP | Deg. F | 88 | 93 | 98 |
| | 5% | Deg. F | 114 | 116 | 119 |
| | 10% | Deg. F | 126 | 123 | 126 |
| | 15% | Deg. F | 134 | 129 | 131 |
| | 20% | Deg. F | 143 | 134 | 137 |
| | 30% | Deg. F | 162 | 144 | 146 |
| | 40% | Deg. F | 188 | 153 | 156 |
| | 50% | Deg. F | 219 | 180 | 163 |
| | 60% | Deg. F | 247 | 237 | 213 |
| | 70% | Deg. F | 272 | 264 | 261 |
| | 80% | Deg. F | 300 | 293 | 290 |
| | 90% | Deg. F | 338 | 333 | 326 |
| | 95% | Deg. F | 368 | 365 | 360 |
| | FBP | Deg. F | 427 | 417 | 421 |
| | Recovered | mL | 99 | 98 | 99 |
| | Residue | mL | 0.9 | 1.1 | 0.7 |
| | Loss | mL | 0.6 | 0.8 | 0.6 |
| D86 | Driveability Index | -- | 1183.5 | 1058.1 | 1002.1 |
| D5191 | Vapor Pressure (Mini Method) | | | | |
| | RVP (EPA Equation) | psi | 8.71 | 9.39 | 9.36 |
| | DVPE (ASTM Equation) | psi | 8.59 | 9.28 | 9.25 |
| D240 | Heat of Combustion | | | | |
| | GROSS | BTU/lb | 19762 | 18566 | 18569 |
| | GROSS | MJ/kg | 45.965 | 43.185 | 43.191 |
| | GROSS | cal/g | 10978.6 | 10314.4 | 10316.1 |
| D240 | Heat of Combustion | | | | |
| | NET | BTU/lb | 18564 | 17380 | 17381 |
| | NET | MJ/kg | 43.181 | 40.426 | 40.428 |
| | NET | cal/g | 10313.6 | 9655.6 | 9656.1 |
| D2622 | Sulfur by X-ray | ppm | - | 4.64 | 4.86 |
| D2699 | Research Octane Number (RON) | -- | 93.0 | 96.2 | 97.6 |
| D2700 | Motor Octane Number (MON) | -- | 83.3 | 85.5 | 86.4 |
| D381 | Existent Gums Content | | | | |
| | Unwashed Wt | mg/100 mL | 5.5 | n/a | n/a |
| | Washed Wt | mg/100 mL | <0.5 | n/a | n/a |
| D4052 | API Gravity | -- | 56.8 | 55.4 | 55.0 |
| | Specific Gravity | -- | 0.7513 | 0.7570 | 0.7586 |
| | Density @ 15°C | g/mL | 0.7510 | 0.7568 | 0.7583 |
| D4815 | Oxygenates and Oxygen Content | | | | |
| | Methanol (MeOH) | vol% | <0.2 | - | - |
| | Ethanol (EtOH) | vol% | <0.2 | - | - |
| | Isopropanol (iPA) | vol% | <0.2 | - | - |
| | tert-Butanol (tBA) | vol% | <0.2 | - | - |
| | n-Propanol (nPA) | vol% | <0.2 | - | - |
| | Methyl tert-butylether (MTBE) | vol% | <0.2 | - | - |
| | sec-Butanol (sBA) | vol% | <0.2 | - | - |
| | Diisopropylether (DIPE) | vol% | <0.2 | - | - |
| | Isobutanol (iBA) | vol% | <0.2 | - | - |
| | Ethyl tert-butylether (ETBE) | vol% | <0.2 | - | - |
| | tert-Pentanol (tPA) | vol% | <0.2 | - | - |
| | n-Butanol (nBA) | vol% | <0.2 | - | - |
| | tert-amyl methylether (TAME) | vol% | <0.2 | - | - |
| | Ethanol (EtOH) | wt% | <0.2 | - | - |
| | Total Oxygen | wt% | 0 | - | - |
| D5291 | Carbon Content | wt% | 86.88 | 83.08 | 81.12 |
| | Hydrogen Content | wt% | 13.12 | 13.00 | 13.02 |
| D5453 | Sulfur by UV | ppm | 4.1 | 4.6 | 4.9 |
| D5599 | Oxygenates and Oxygen Content | | | | |
| | Diisopropylether (DIPE) | vol% | n/a | <0.1 | <0.1 |
| | Ethyl tert-butylether (ETBE) | vol% | n/a | <0.1 | <0.1 |
| | Ethanol (EtOH) | vol% | n/a | 10.07 | 15.09 |
| | Ethanol (EtOH) | WT% | n/a | 10.56 | 15.80 |
| | Isobutanol (iBA) | vol% | n/a | <0.1 | <0.1 |
| | Isopropanol (iPA) | vol% | n/a | <0.1 | <0.1 |
| | Methanol (MeOH) | vol% | n/a | <0.1 | <0.1 |
| | Methyl tert-butylether (MTBE) | vol% | n/a | <0.1 | <0.1 |
| | n-Butanol (nBA) | vol% | n/a | <0.1 | <0.1 |
| | n-Propanol (nPA) | vol% | n/a | <0.1 | <0.1 |
| | sec-Butanol (sBA) | vol% | n/a | <0.1 | <0.1 |
| | tert-amyl methylether (TAME) | vol% | n/a | <0.1 | <0.1 |
| | tert-Butanol (tBA) | vol% | n/a | <0.1 | <0.1 |
| | tert-Pentanol (tPA) | vol% | n/a | <0.1 | <0.1 |
| | Total Oxygen | WT% | n/a | 3.67 | 5.48 |

EM-10967-F



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Certificate of Analysis

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PRODUCT: **EPA Tier 3 EEE**
Emission Certification Fuel,
General Testing - Regular
 Specification No.: **HF2021**

Batch No.: **HH2921LT10-10**Tank No.: **TK107**Date: **10/10/2019**

| TEST | METHOD | UNITS | SPECIFICATIONS | | | RESULTS |
|-------------------------------------|----------------------------|-------------|----------------|--------|--------|---------------|
| | | | MIN | TARGET | MAX | |
| Distillation - IBP | ASTM D86 ² | °F | | | | 96.5 |
| 5% | | °F | | | | 120.2 |
| 10% | | °F | 120 | | 140 | 129.0 |
| 20% | | °F | | | | 138.5 |
| 30% | | °F | | | | 147.3 |
| 40% | | °F | | | | 154.3 |
| 50% | | °F | 190 | | 210 | 195.1 |
| 60% | | °F | | | | 233.2 |
| 70% | | °F | | | | 256.0 |
| 80% | | °F | | | | 282.0 |
| 90% | | °F | 315 | | 335 | 322.2 |
| 95% | | °F | | | | 341.5 |
| Distillation - EP | | °F | 380 | | 420 | 387.7 |
| Recovery | | % | | Report | | 97.1 |
| Residue | | ml | | | 2.0 | 0.8 |
| Loss | | % | | Report | | 2.1 |
| Gravity @ 60° F | ASTM D4052 ² | °API | | Report | | 58.90 |
| Density @ 15.56° C | ASTM D4052 ² | kg/l | | Report | | 0.7425 |
| Raid Vapor Pressure EPA Equation | ASTM D5191 ² | psi | 8.7 | | 9.2 | 9.2 |
| Carbon | ASTM D5291 ² | wt fraction | | Report | | 0.8239 |
| Hydrogen | ASTM D5291 ² | wt fraction | | Report | | 0.1387 |
| Hydrogen/Carbon ratio | ASTM D5291 ² | mole/mole | | Report | | 2.006 |
| Oxygen | ASTM D4815 ² | wt % | | Report | | 3.74 |
| Ethanol content | ASTM D5599-00 ² | vol % | 9.6 | | 10.0 | 9.7 |
| Total oxygenates other than ethanol | ASTM D4815 ² | vol % | | 0.1 | | None Detected |
| Sulfur | ASTM D5453 ² | mg/kg | 8.0 | | 11.0 | 9.2 |
| Phosphorus | ASTM D3231 ² | g/l | | | 0.0013 | None Detected |
| Lead | ASTM D3237 ² | g/l | | | 0.0026 | None Detected |
| Composition, aromatics | ASTM D5769 ¹ | vol % | 21.0 | | 26.0 | 22.2 |
| C6 aromatics (benzene) | ASTM D5769 ¹ | vol % | 0.5 | | 0.7 | 0.6 |
| C7 aromatics (toluene) | ASTM D5769 ¹ | vol % | 5.2 | | 6.4 | 5.6 |
| C8 aromatics | ASTM D5769 ¹ | vol % | 9.2 | | 6.4 | 5.3 |
| C9 aromatics | ASTM D5769 ¹ | vol % | 5.2 | | 6.4 | 5.5 |
| C10+ aromatics | ASTM D5769 ¹ | vol % | 4.4 | | 5.6 | 5.0 |
| Composition, olefins | ASTM D6550 ² | wt % | 4.0 | | 10.0 | 7.0 |
| Oxidation Stability | ASTM D525 ² | minutes | 1000 | | | 1000+ |
| Copper Corrosion | ASTM D130 ² | | | | 1 | 1a |
| Existent gum, washed | ASTM D381 ² | mg/100mls | | | 3.0 | 1.0 |
| Existent gum, unwashed | ASTM D381 ² | mg/100mls | | Report | | 2.0 |
| Research Octane Number | ASTM D2699 ² | | | Report | | 92.3 |
| Motor Octane Number | ASTM D2700 ² | | | Report | | 84.5 |
| R+M/2 | D2699/2700 ² | | 87.0 | | 88.4 | 88.4 |
| Sensitivity | D2699/2700 ² | | 7.5 | | | 7.8 |
| Net Heat of Combustion | ASTM D240 ² | BTU/lb | | Report | | 17914 |

Quality Assurance Technician

¹ Haltermann Solutions is accredited to ISO/IEC 17025 by ANAB for the tests referred to with this footnote.



² Tested by ISO/IEC 17025 accredited subcontractor.

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Page 1 of 1

APPENDIX B

DETAILED TEST PROCEDURES

Fuel Change Procedure

1. Drain vehicle fuel completely via fuel rail whenever possible.
2. Turn vehicle ignition to RUN position for 30 seconds allowing fuel level reading to stabilize. Confirm the return of fuel gauge reading to zero.
3. Turn ignition off. Fill fuel tank to 40% with next test fuel in sequence. Fill-up fuel temperature must be less than 50°F.
4. Start vehicle and execute catalyst sulfur removal procedure described in Appendix B. Apply side fan cooling to the fuel tank to alleviate the heating effect of the exhaust system. Engine oil temperature in the sump will be measured and recorded during the sulfur removal cycle.
5. Perform four vehicle coast downs from 70 to 30 mph, with the last two measured. The vehicle will be checked for any obvious and gross source of change in the vehicle's mechanical friction if the individual run fails to meet the following repeatability criteria: 1) maximum difference of 0.5 seconds between back-to-back coastdown runs from 70 to 30 mph; and 2) maximum ± 7 percent difference in average 70 to 30 mph coastdown time from the running average for a given vehicle.
6. Drain fuel and refill to 40% with test fuel. Fill-up fuel should be at approximately 50°F.
7. Drain fuel again and refill to 40% with test fuel. Fill-up fuel should be at approximately 50°F.
8. Soak vehicle for at least 12 hours to allow fuel temperature to stabilize to the test temperature.

Catalyst Sulfur Purge Cycle

This procedure is designed to cause the vehicle to transiently run rich at high catalyst temperature, to remove accumulated sulfur from the catalyst, via hydrogen sulfide formation. The catalyst inlet temperature will be monitored during this procedure. It is required to demonstrate that the catalyst inlet temperature exceeds 700°C during the WOT accelerations and that rich fuel/air mixtures are achieved during WOT. If these parameters are not achieved, increased loading on the dynamometer could be added for this protocol (but not during the emissions test). Increased loading is not included in this proposal.

1. Drive the vehicle from idle to 55 mph and hold speed for 5 minutes (to bring catalyst to full working temperature).
2. Reduce vehicle speed to 30 mph and hold speed for one minute.
3. Accelerate at WOT (wide-open throttle) for a minimum of 5 seconds, to achieve a speed greater than 70 mph. Continue WOT above 70 mph, if necessary to achieve 5-second acceleration duration. Hold the peak speed for 15 seconds and then decelerate to 30 mph.
4. Maintain 30 mph for one minute.
5. Repeat steps 3 and 4 to achieve 5 WOT excursions.
6. One sulfur removal cycle has been completed.
7. Repeat steps 1 to 5 for the second sulfur removal cycle.
8. The protocol is complete if the necessary parameters have been achieved.

Vehicle Conditioning

1. Move vehicle to test area without starting engine. Start vehicle and perform the EPA Urban Dynamometer Driving Schedule (UDDS) followed by two Highway Fuel Economy Driving Schedules (HWFET) followed by a US06 Supplemental FTP Driving Schedule (US06) test. During the prep cycle, apply side fan cooling to the fuel tank to alleviate the heating effect of the exhaust system. Following the first two prep cycles, allow vehicle to idle in park for two minutes, then shut-down the engine for 2-5 minutes. Following the last prep cycle, allow the vehicle to idle for two minutes, then shut down the engine in preparation for the soak.
2. Move vehicle to test area without starting engine.
3. Park vehicle in soak area at proper temperature (75 °F) for 12-36 hours. During the soak period, maintain the nominal charge of the vehicle's battery using an appropriate charging device.
4. Move vehicle to test area without starting engine.
5. Conduct LA-92 prep cycle and then soak vehicle for 12-36 hours.

APPENDIX C

Test results are provided in a separate file
CRC RW-107-3 Results Appendix C.csv

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 | 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 | C7H16 | 49.4 | 2.0 | experiment | 662.8 |
| 2-Methylheptane | 592-27-8 | 11594 | 2-methylheptane | CCCCC(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 | CCCC=CC | C7H14 | 54.4 | 9.1 | prediction | 544.6 |
| c-Heptene-2 | | 643836 | (Z)-hept-2-ene | CCCC=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 | CCCC=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 | CCCC(C)CC=C | C7H14 | 55.8 | 2.0 | experiment | 731.7 |
| 4-Methylhexene-1 | | 19589 | 4-methylhex-1-ene | CCCC(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 | CCCCC(=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 | CCCCC(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 | CCCC(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 | CCCC(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 | CCCCC(C)(C)C | C9H20 | 62.6 | 9.0 | prediction | 252.6 |
| 3,3-Diethylpentane | 1067-20-5 | 14020 | 3,3-diethylpentane | CC(C)(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 | CCCCC(C)(C)C | C9H20 | 62.6 | 9.0 | prediction | 255.3 |
| Heptane, 2,2-dimethyl- | | 14062 | 2,2-dimethylheptane | CCCCC(C)(C)C | C9H20 | 62.6 | 9.0 | prediction | 252.6 |
| Heptane, 3,3-dimethyl- | | 520991 | 3,3-dimethylheptane | CCCC(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 | CCC(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-Ethyl-octane | 5881-17-4 | 79985 | 3-ethyl-octane | CCCCC(C)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 | CCCCC(C)CCC | C10H22 | 64.1 | 8.8 | prediction | 111.0 |
| 5-Methylnonane | 15869-85-9 | 27518 | 5-methylnonane | CCCC(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 | CCCCC(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 | 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 | CCCCCC=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 | CCCCC=CCC | C9H18 | 67.5 | 9.1 | prediction | 227.3 |
| cis-4-Nonene | 10405-84-2 | 5364456 | (Z)-non-4-ene | CCCC=CCCC | C9H18 | 67.5 | 9.1 | prediction | 181.9 |
| c-Nonene-2 | | 5364455 | (Z)-non-2-ene | CCCCC=CC | C9H18 | 67.5 | 9.1 | prediction | 162.1 |
| c-Nonene-3 | 20237-46-0 | 5364453 | (Z)-non-3-ene | CCCCC=CCC | C9H18 | 67.5 | 9.1 | prediction | 227.3 |
| t-Nonene-2 | 6434-78-2 | 5364590 | (E)-non-2-ene | CCCCC=CC | C9H18 | 67.5 | 9.1 | prediction | 189.5 |
| t-Nonene-3 | 20063-92-7 | 5364445 | (E)-non-3-ene | CCCCC=CCC | C9H18 | 67.5 | 9.1 | prediction | 181.9 |
| trans-4-Nonene | 10405-85-3 | 5364454 | (E)-non-4-ene | CCCC=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 | CC1CCCC(C1)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 | 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 | 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 | C9H20 | 68.4 | 9.0 | prediction | 302.8 |
| C9 - MonoNaph - 5 | | 28022 | 2,2,4-trimethylhexane | CCC(C)CC(C)C | C9H20 | 68.4 | 9.0 | prediction | 196.8 |
| C9_I-Paraffins(1) | | 19041 | 2,2,5-trimethylhexane | CC(C)CCC(C)C | C9H20 | 68.4 | 9.0 | prediction | 245.9 |
| C9_I-Paraffins(5) | | 19041 | 2,2,5-trimethylhexane | CC(C)CCC(C)C | C9H20 | 68.4 | 9.0 | prediction | 261.7 |
| C9_I-Paraffins(6) | | 19041 | 2,2,5-trimethylhexane | CC(C)CCC(C)C | C9H20 | 68.4 | 9.0 | prediction | 276.5 |
| C9-Isoparaffin-x | | 19041 | 2,2,5-trimethylhexane | CC(C)CCC(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 | C9H20 | 68.4 | 9.0 | prediction | 219.1 |
| Hexane, 2,4,4-trimethyl- | 16747-30-1 | 28024 | 2,4,4-trimethylhexane | CCC(C)C(C)C | C9H20 | 68.4 | 9.0 | prediction | 276.5 |
| Hexane, 3,3,4-trimethyl- | | 28025 | 3,3,4-trimethylhexane | CCC(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 | 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 | C8H16 | 68.5 | 2.1 | experiment | 504.8 |
| C8 - IsoOlefin - 10 | | 7868 | 2,4,4-trimethylpent-1-ene | CC(=C)CC(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 | C8H16 | 68.5 | 2.1 | experiment | 363.7 |
| C8 - IsoOlefin - 5 | | 7868 | 2,4,4-trimethylpent-1-ene | CC(=C)CC(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 | 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 |

| 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-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 | CCCCC(C)C(C)C | C10H22 | 69.9 | 9.0 | prediction | 148.3 |
| 2,3-Dimethyloctane(1) | | 23531 | 2,3-dimethyloctane | CCCCC(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)CCCC(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 | CCCCC(C)C(C)C | C10H22 | 69.9 | 9.0 | prediction | 118.9 |
| C10_I-Paraffins(14) | | 23531 | 2,3-dimethyloctane | CCCCC(C)C(C)C | C10H22 | 69.9 | 9.0 | prediction | 118.9 |
| C10_I-Paraffins(15) | | 23531 | 2,3-dimethyloctane | CCCCC(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(C)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 | CCCCC(C)CCCC | C11H24 | 70.7 | 8.9 | prediction | 71.9 |
| C11_I-Paraffins(15) | | 93071 | 5-methyldecane | CCCCC(C)CCCC | C11H24 | 70.7 | 8.9 | prediction | 70.6 |
| C11_I-Paraffins(16) | | 93071 | 5-methyldecane | CCCCC(C)CCCC | C11H24 | 70.7 | 8.9 | prediction | 70.6 |
| C11_I-Paraffins(17) | | 93071 | 5-methyldecane | CCCCC(C)CCCC | C11H24 | 70.7 | 8.9 | prediction | 70.6 |
| C11_I-Paraffins(18) | | 93071 | 5-methyldecane | CCCCC(C)CCCC | C11H24 | 70.7 | 8.9 | prediction | 70.6 |
| C11_I-Paraffins(19) | | 23415 | 2-methyldecane | CCCCCCCC(C)C | C11H24 | 70.7 | 8.9 | prediction | 70.6 |
| C11_I-Paraffins(20) | | 23415 | 2-methyldecane | CCCCCCCC(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 | CCCCCCCC(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 | CCCCC(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 | 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 | CCCCC=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 | CCCCC=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 | CCCC(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 | CCCCC=C(C)C | C9H18 | 75.6 | 9.1 | prediction | 176.3 |
| 2-Methyloctene-2 | 16993-86-4 | 140163 | 2-methyloct-2-ene | CCCCC=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 | C10H22 | 75.8 | 9.2 | prediction | 138.8 |
| C10_I-Paraffins(10) | | 19944 | 2,3,6-trimethylheptane | CC(C)CCC(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 | C10H22 | 75.8 | 9.2 | prediction | 127.4 |
| C10_I-Paraffins(2) | | 140667 | 2,3,5-trimethylheptane | CCC(C)CC(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 | C10H22 | 75.8 | 9.2 | prediction | 138.8 |
| C10_I-Paraffins(4) | | 140667 | 2,3,5-trimethylheptane | CCC(C)CC(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 | C10H22 | 75.8 | 9.2 | prediction | 138.8 |
| C10_I-Paraffins(9) | | 19944 | 2,3,6-trimethylheptane | CC(C)CCC(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 | 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,2à,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-, (1à,2B,4à)- | | 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)CCC | C11H24 | 76.5 | 9.0 | prediction | 70.6 |
| C11_I-Paraffins(25) | | 86541 | 4,5-dimethylnonane | CCCCC(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 | 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)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 | CCCC1CCCC1 | C10H20 | 76.8 | 2.2 | experiment | 77.4 |
| n-ButylCyclohexane | 1678-93-9 | 15506 | butylcyclohexane | CCCC1CCCC1 | 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(C1)C | C9H18 | 76.9 | 9.3 | prediction | 160.8 |
| 1-Ethyl-4-methylcyclohexane | 3728-56-1 | 19503 | 1-ethyl-4-methylcyclohexane | CCC1CCC(C1)C | C9H18 | 76.9 | 9.3 | prediction | 160.9 |
| 1-ethyl-4-t-methylcyclohexane | | 19503 | 1-ethyl-4-methylcyclohexane | CCC1CCC(C1)C | C9H18 | 76.9 | 9.3 | prediction | 161.8 |
| C9_Mono-Naphthenes(20) | | 19503 | 1-ethyl-4-methylcyclohexane | CCC1CCC(C1)C | C9H18 | 76.9 | 9.3 | prediction | 160.9 |
| C9_Mono-Naphthenes(22) | | 19503 | 1-ethyl-4-methylcyclohexane | CCC1CCC(C1)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 | CCCC1CCCC(C1)C | C9H18 | 76.9 | 9.3 | prediction | 160.9 |
| Cyclohexane, 1-ethyl-2-methyl- | | 35413 | 1-ethyl-2-methylcyclohexane | CCC1CCCC1C | C9H18 | 76.9 | 9.3 | prediction | 160.9 |
| Cyclohexane, 1-ethyl-2-methyl-, cis- | 4923-77-7 | 23620236 | (1S,2R)-1-ethyl-2-methylcyclohexane | CCC1CCCC1C | 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(C1)C | C9H18 | 76.9 | 9.3 | prediction | 168.7 |
| Cyclohexane, 1-ethyl-4-methyl-, trans- | 6236-88-0 | 19503 | 1-ethyl-4-methylcyclohexane | CCC1CCC(C1)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)C)C | C8H16 | 77.1 | 10.0 | prediction | 317.9 |
| 5-Ethyldecane | | 529848 | 5-ethyldecane | CCCCC(C)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(C)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(C)CCC | C12H26 | 77.3 | 8.9 | prediction | 46.1 |
| C12_I-Paraffins(8) | | 519256 | 4-ethyldecane | CCCCCCC(C)CCC | C12H26 | 77.3 | 8.9 | prediction | 50.4 |
| C12_I-Paraffins(9) | | 519256 | 4-ethyldecane | CCCCCCC(C)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(C)CCC | C12H26 | 77.3 | 8.9 | prediction | 46.1 |
| Decane, 4-ethyl- | 1636-44-8 | 519256 | 4-ethyldecane | CCCCCCC(C)CCC | C12H26 | 77.3 | 8.9 | prediction | 46.1 |
| Undecane, 2-methyl- | 7045-71-8 | 23459 | 2-methylundecane | CCCCCCCC(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 | CCCCCCCCCCCC | C14H30 | 78.4 | 3.9 | experiment | 12.0 |
| n-Tetradecane | 629-59-4 | 12389 | tetradecane | CCCCCCCCCCCC | 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)CCC=C(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)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)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 | CCCCCCC=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)CC=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 | CCCCC(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 | CCCCC(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 | CCCCC(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 | CCCCC(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 | C9H18 | 82.0 | 9.4 | prediction | 197.1 |
| Cyclopentane, 1-methyl-3-(1-methylethyl)- | | 521465 | 1-methyl-3-propan-2-ylcyclopentane | CC1CCC(C1)(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 | 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 | CCCCC=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(C)C(C)C | C11H24 | 82.3 | 9.3 | prediction | 85.1 |
| C11_I-Paraffins(10) | | 545571 | 2,5,6-trimethyloctane | CCC(C)(C)C(C)C(C)C | C11H24 | 82.3 | 9.3 | prediction | 79.3 |
| C11_I-Paraffins(11) | | 545571 | 2,5,6-trimethyloctane | CCC(C)(C)C(C)C(C)C | C11H24 | 82.3 | 9.3 | prediction | 79.3 |
| C11_I-Paraffins(12) | | 545571 | 2,5,6-trimethyloctane | CCC(C)(C)C(C)C(C)C | C11H24 | 82.3 | 9.3 | prediction | 70.6 |
| C11_I-Paraffins(13) | | 545571 | 2,5,6-trimethyloctane | CCC(C)(C)C(C)C(C)C | C11H24 | 82.3 | 9.3 | prediction | 70.6 |
| C11_I-Paraffins(14) | | 545571 | 2,5,6-trimethyloctane | CCC(C)(C)C(C)C(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 | 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 | 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 | CCCCCCC(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 | CCCCC1CCCCC1 | C11H22 | 83.5 | 9.0 | prediction | 85.9 |
| C11 - MonoNaph - 2 | | 20284 | pentylcyclohexane | CCCCC1CCCCC1 | C11H22 | 83.5 | 9.0 | prediction | 59.9 |
| C11 - MonoNaph - 3 | | 20284 | pentylcyclohexane | CCCCC1CCCCC1 | C11H22 | 83.5 | 9.0 | prediction | 46.9 |
| C11_Mono-Naphthenes(1) | | 20284 | pentylcyclohexane | CCCCC1CCCCC1 | C11H22 | 83.5 | 9.0 | prediction | 70.6 |
| C11_Mono-Naphthenes(2) | | 20284 | pentylcyclohexane | CCCCC1CCCCC1 | 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 | CC1CCC(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 |
| Diethylcyclohexane | | 14910 | 1,4-diethylcyclohexane | CC1CCC(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(C1)C | C9H18 | 83.6 | 10.2 | prediction | 168.5 |
| Cyclohexane, 1,3,5-trimethyl-, (1à,3à,5à)- | 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,5β)- | | 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(C)CCCC | C13H28 | 83.9 | 8.9 | prediction | 17.5 |
| C13_I-Paraffins(4) | | 519397 | 3-ethylundecane | CCCCCCCC(C)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 | CCCCCCCC(C)CC | C13H28 | 83.9 | 8.9 | prediction | 20.8 |
| Undecane, 5-ethyl- | | 519424 | 5-ethylundecane | CCCCCCC(C)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 | 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 |

| 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_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-trimethyl | 72014-90-5 | 522437 | 2,3,4-trimethylpenta-1,4-diene | CC(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 | 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)CCCC=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 | C11H24 | 87.4 | 9.2 | prediction | 30.8 |
| C11 - IsoParaffin - 6 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 67.4 |
| C11- Isoparaffin - 12 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 61.4 |
| C11 Isoparaffin - 4 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 87.7 |
| C11 Isoparaffin-1 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 68.3 |
| C11- Isoparaffin-11 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 97.5 |
| C11 Isoparaffin-4 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | 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 | 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 | 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 | 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 | C11H24 | 87.4 | 9.2 | prediction | 71.8 |
| C11-Isoparaffin-1 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 119.3 |
| C11-Isoparaffin-3 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 82.6 |
| C11-Isoparaffin-7 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | C11H24 | 87.4 | 9.2 | prediction | 66.7 |
| C11-Isoparaffin-9 | | 545795 | 2,2,3,5-tetramethylheptane | CCC(C)CC(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 | 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,2à,3à,4à-Tetramethylcyclopentane | 2532-67-4 | 137631 | 1,2,3,4-tetramethylcyclopentane | CC1CC(C(C1C)C)C | C9H18 | 89.4 | 11.7 | prediction | 234.6 |
| 1à,2à,3à,4à-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)CCCCC(C)C | C13H28 | 89.7 | 9.0 | prediction | 25.4 |
| Undecane, 2,7-dimethyl- | 17301-24-5 | 519383 | 2,7-dimethylundecane | CCCCC(C)CCCC(C)C | C13H28 | 89.7 | 9.0 | prediction | 25.0 |
| Undecane, 2,8-dimethyl- | 17301-25-6 | 519384 | 2,8-dimethylundecane | CCCC(C)CCCCC(C)C | C13H28 | 89.7 | 9.0 | prediction | 25.0 |
| Cyclohexane, 1-ethyl-2,3-dimethyl- | 1884043 | 550319 | 1-ethyl-2,3-dimethylcyclohexane | CC(C1CCCC(C1)C)C | C10H20 | 90.1 | 10.2 | prediction | 113.0 |
| 2,3-Dimethyl-2-octene | | 140599 | 2,3-dimethyloct-2-ene | CCCCC(C=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)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 |

| Compound Name (as it appears in DHA) | CAS NO | CID | IUPAC Name | Canonical SMILES | Molecular Formula | YSI | YSI Error | Prediction Type | VP _{443K} (kPa) |
|--|------------|----------|--|------------------------|-------------------|-------|-----------|-----------------|--------------------------|
| 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-(1-methylethyl)- | | 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)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 19.3 |
| C13 - IsoParaffin - 2 | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 17.4 |
| C13 - IsoParaffin - 6 | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 11.5 |
| C13 - IsoParaffin - 7 | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 10.2 |
| C13_I-Paraffins(1) | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 17.5 |
| C13_I-Paraffins(6) | | 522039 | 2,3,5-trimethyldecane | CCCCC(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)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 64.1 |
| C13_I-Paraffins(8) | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(C)C(C)C | C13H28 | 95.5 | 9.3 | prediction | 70.6 |
| C13_I-Paraffins(9) | | 545623 | 2,3,8-trimethyldecane | CCC(C)CCCC(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 | CCCCC(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)CCCC(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-methylenecyclobutane | 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(CCC(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(=C1CCCC1)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 | C1CCCC2CCCCC2C1 | 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 | CCCCC1(CCCCC1)CC | C13H26 | 108.5 | 11.5 | prediction | 40.7 |
| C13-Mono-Naphthene-1 | | 21657239 | 1-ethyl-1-pentylcyclohexane | CCCCC1(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 | CCCC#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 | 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=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=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=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 | CC1CCCC(=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 | CC12CCCC1CCCC2 | 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 | CCCCCCC2C1(CCCC2)C | C12H22 | 124.9 | 11.4 | prediction | 9.1 |
| Cyclopentane, 1,3-bis(methylene)- | | 556487 | 1,3-dimethylenecyclopentane | 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 | CCCCC1(CC1)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(=C1)C | C8H14 | 140.8 | 15.5 | prediction | 318.3 |
| Cyclopentene, 1,2,3-trimethyl- | 473-91-6 | 136316 | 1,2,3-trimethylcyclopentene | CC1CCC(=C1)C | C8H14 | 140.8 | 15.5 | prediction | 329.9 |
| 1,3-Cyclopentadiene, 1,2-dimet | | 0 | unknown | CC1=C(C=C1)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 | CCCC1=CC=CC=C1 | C10H14 | 245.1 | 9.9 | experiment | 71.8 |
| n-Hexylbenzene | 1077-16-3 | 14109 | hexylbenzene | CCCCCC1=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 | CCCCC1=CC=CC=C1 | C11H16 | 255.0 | 10.5 | experiment | 40.3 |
| s-Pentylbenzene | | 10864 | pentylbenzene | CCCCC1=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)CC1=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 | CCCC1=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 | CCCCCCC1=CC=C(C=C1)C | C12H18 | 300.1 | 9.7 | prediction | 22.5 |
| C12_Mono-Aromatics(5) | | 524159 | 1-methyl-4-pentylbenzene | CCCCCCC1=CC=C(C=C1)C | C12H18 | 300.1 | 9.7 | prediction | 41.8 |
| C12_Mono-Aromatics(6) | | 524159 | 1-methyl-4-pentylbenzene | CCCCCCC1=CC=C(C=C1)C | C12H18 | 300.1 | 9.7 | prediction | 41.8 |
| Benzene, (1,1-dimethylbutyl)- | | 16136 | 2-methylpentan-2-ylbenzene | CCC(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-(1-methylethyl)- | | 20833 | 1,3-dimethyl-5-propan-2-ylbenzene | CC1=CC(=CC=C1)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(=C(C=C1)C(C)C | C11H16 | 339.9 | 14.0 | prediction | 54.6 |
| Benzene, 1,4-dimethyl-2-(1-methylethyl)- | | 77784 | 1,4-dimethyl-2-propan-2-ylbenzene | CC1=CC(=C(C=C1)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 | C11H16 | 339.9 | 14.0 | prediction | 51.4 |
| Benzene, 2,4-dimethyl-1-(1-methylethyl)- | | 20832 | 2,4-dimethyl-1-propan-2-ylbenzene | CC1=CC(=C(C=C1)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 | 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 | 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 | 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 | C11H16 | 339.9 | 14.0 | prediction | 56.2 |
| 1,2-Dimethyl-3-ethylbenzene | 933-98-2 | 13621 | 1-ethyl-2,3-dimethylbenzene | CC1=CC=CC(=C1)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=C1)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 | 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=C1)C | C10H14 | 341.6 | 10.7 | prediction | 60.3 |
| C10_Mono-Aromatics(7) | | 17877 | 2-ethyl-1,3-dimethylbenzene | CCC1=C(C=CC=C1)C | C10H14 | 341.6 | 10.7 | prediction | 60.5 |
| Benzene, 2,4-dimethyl-1-(1-methylpropyl)- | | 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)-3-methyl- | | 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-(2-methylpropyl)- | | 41508 | 1,4-dimethyl-2-(2-methylpropyl)benzene | CC1=CC(=C(C=C1)C)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)C)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)C)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)C)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 | 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=C1)C)C | C10H14 | 393.0 | 15.3 | experiment | 51.7 |
| Benzene, 1,2,4-trimethyl-5-(1-methylethyl)- | | unknown | unknown | CC1=CC(=C(C=C1)C(C)C | C12H18 | 401.2 | 15.1 | prediction | 27.8 |
| C12_Mono-Aromatics(17) | | 0 | unknown | CC1=CC(=C(C=C1)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(C=C1)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 | CCC=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=C(C(=C1)C)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(=C1)C)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(=C1)C)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(=C1)C)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 | 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 | 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-(1-methylethyl)- | | 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-(1-methylethyl)- | | 16952 | 1-propan-2-yl-4-prop-1-en-2-ylbenzene | CC(C)C1=CC=C(C(=C1)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 | 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(CCC2=CC=CC=C2)C | C11H14 | 420.8 | 19.9 | prediction | 45.2 |
| C14_Mono-Aromatics(1) | | 90961365 | 1,2,5-trimethyl-3-pentylbenzene | CCCCCCC1=CC(=CC(=C1)C)C | C14H22 | 422.7 | 12.3 | prediction | 4.3 |
| C14_Mono-Aromatics(2) | | 90961365 | 1,2,5-trimethyl-3-pentylbenzene | CCCCCCC1=CC(=CC(=C1)C)C | C14H22 | 422.7 | 12.3 | prediction | 9.0 |
| C14_Mono-Aromatics(3) | | 90961365 | 1,2,5-trimethyl-3-pentylbenzene | CCCCCCC1=CC(=CC(=C1)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=C2)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=C2)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=C2)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=C2)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=C2CC(CCC2=CC=C1)C | 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(=C1)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=C2 | C9H8 | 467.7 | 17.8 | experiment | 247.4 |
| Indene | 95-13-6 | 7219 | 1H-indene | C1C=CC2=CC=CC=C2 | 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-1H-Indene, 1-methyl- | 767-59-9 | 522578 13024 | 2,6-dimethyl-1,2,3,4-tetrahydronaphthalene 1-methyl-1H-indene | CC1CCC2=C(C1)C=CC(=C2)C CC1C=CC2=CC=CC=C12 | C12H16 C10H10 | 471.0 479.1 | 18.7 32.9 | prediction outlier | 12.0 56.5 |
| 1H-Indene, 3-methyl-C10_Indenes(1) | 767-59-9 | 13024 13024 | 1-methyl-1H-indene 1-methyl-1H-indene | CC1C=CC2=CC=CC=C12 CC1C=CC2=CC=CC=C12 | C10H10 C10H10 | 479.1 479.1 | 32.9 32.9 | outlier outlier | 40.1 56.5 |
| α,β,β-Trimethylstyrene | | 13036 | 2-ethenyl-1,3,5-trimethylbenzene | CC1=CC(=C(C(=C1)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(=C1)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-n-propyl indane | 92013-16-6 | 583029 13330218 | 4-propyl-2,3-dihydro-1H-indene 5-propyl-2,3-dihydro-1H-indene | CCCC1=CC=CC2=C1CCC2 CCCC1=CC2=C(CCCC2)C=C1 | C12H16 C12H16 | 488.0 488.0 | 19.1 19.1 | prediction prediction | 11.8 18.3 |
| 5-Ethyltetralin | | 54756 | 5-ethyl-1,2,3,4-tetrahydronaphthalene | CC1C=CC2=CC=C1CCC2 | 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-1H-Indene, 2,3-dihydro-1,1,5-trimethyl-1H-Indene, 2,3-dihydro-1,1,6-trimethyl-C12_Indanes(2) | 16204-72-1 40650-41-7 | 589442 589447 589441 589442 | 3,3,7-trimethyl-1,2-dihydroindene 3,3,6-trimethyl-1,2-dihydroindene 3,3,5-trimethyl-1,2-dihydroindene 3,3,7-trimethyl-1,2-dihydroindene | CC1=C2CCC(C2=CC=C1)(C)C CC1=C2CCC(C2=CC=C1)(C)C CC1=CC2=C(CCC2(C)C)C=C1 CC1=C2CCC(C2=CC=C1)(C)C | C12H16 C12H16 C12H16 C12H16 | 489.4 489.4 489.4 489.4 | 17.6 17.6 17.6 17.6 | outlier outlier outlier outlier | 13.5 12.8 13.5 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-C13_Indanes(1) | 767-58-8 | 13023 297000 | 1-methyl-2,3-dihydro-1H-indene 6-propyl-1,2,3,4-tetrahydronaphthalene | CC1CCC2=CC=CC=C12 CCCC1=CC2=C(CCCC2)C=C1 | C10H12 C13H18 | 492.4 495.3 | 26.3 19.1 | prediction prediction | 55.3 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-Naphthalene, 1,2,3,4-tetrahydro-6-propyl-1H-Indene, 1-ethyl-2,3-dihydro- | 42775-77-9 4830-99-3 | 297000 20971 | 6-propyl-1,2,3,4-tetrahydronaphthalene 1-ethyl-2,3-dihydro-1H-indene | CCCC1=CC2=C(CCCC2)C=C1 CCC1CCC2=CC=CC=C12 | C13H18 C11H14 | 495.3 499.0 | 19.1 26.3 | prediction prediction | 7.3 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-Naphthalene, 1,2,3,4-tetrahydro-1-methyl-1H-Indene, 2,3-dihydro-1,2-dim | 1559-81-5 | 15262 28225 | 1-methyl-1,2,3,4-tetrahydronaphthalene 1,2-dimethyl-2,3-dihydro-1H-indene | CC1CCCC2=CC=CC=C12 CC1CC2=CC=CC=C2C1C | C11H14 C11H14 | 499.7 505.6 | 26.3 26.6 | prediction prediction | 26.7 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-Naphthalene, 1-ethyl-1,2,3,4-tetrahydro- | | 139497 | 1-ethyl-1,2,3,4-tetrahydronaphthalene | CCC1CCC2=CC=CC=C12 | C12H16 | 506.3 | 26.3 | prediction | 15.5 |
| Naphthalene, 1-ethyl-1,2,3,4-tetrahydro-1H-Indene, 2,3-dihydro-4,6-dimethyl-1H-Indene, 2,3-dihydro-5,6-dimethyl-4,7-Dimethyl Indan | 13556-58-6 1685-82-1 1075-22-5 | 139497 15518 70635 23151 | 1-ethyl-1,2,3,4-tetrahydronaphthalene 4,6-dimethyl-2,3-dihydro-1H-indene 5,6-dimethyl-2,3-dihydro-1H-indene 4,7-dimethyl-2,3-dihydro-1H-indene | CCC1CCCC2=CC=CC=C12 CC1=CC(=C2CCCC2=C1)C CC1=CC2=C(CCC2)C=C1C CC1=C2CCCC2=C(C=C1)C | C12H16 C11H14 C11H14 C11H14 | 506.3 511.8 511.8 511.8 | 26.3 19.2 19.2 19.2 | prediction prediction prediction prediction | 15.5 23.5 21.9 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(C(CCC2)C=C1)C | C12H16 | 519.1 | 19.2 | prediction | 9.9 |
| Naphthalene, 1,2,3,4-tetrahydro-5,6-dimethyl-1,1,3-Trimethyl Indan | 20027-77-4 | 589445 | 5,6-dimethyl-1,2,3,4-tetrahydronaphthalene | CC1=C(C2=C(C(CCC2)C=C1)C | C12H16 | 519.1 | 19.2 | prediction | 9.9 |
| 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 | 17.8 |
| 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 Indane - 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 Indane - 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 Indane - 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 Indane - 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 Indane - 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 Indane - 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 Indane - 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=C12C | C12H16 | 561.0 | 26.5 | prediction | 14.6 |
| C12_Indanes(5) | | 23150 | 4,5,7-trimethyl-2,3-dihydro-1H-indene | CC1=CC(=C2CCCC2=C1)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=C1)C | C12H16 | 573.1 | 20.1 | prediction | 11.8 |
| Indane,4,5,7-trimethyl | 6682-06-0 | 23150 | 4,5,7-trimethyl-2,3-dihydro-1H-indene | CC1=CC(=C2CCCC2=C1)C | C12H16 | 573.1 | 20.1 | prediction | 11.8 |
| 1-H-Indene,1-3-dimethyl | 2177-48-2 | 582329 | 1,3-dimethyl-1H-indene | CC1=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 | CC1CCC2=CC=CC=C12C | 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-ynaphthalene | 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-ynaphthalene | 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=C1C | 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-Ethynaphthalene | 939-27-5 | 13652 | 2-ethynaphthalene | 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-Ethynaphthalene | 1127-76-0 | 14315 | 1-ethynaphthalene | 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 |

