Compendium of Experimental Cetane Numbers

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Ecoengineering

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National Renewable Energy Laboratory

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Based on the *Compendium of Experimental Cetane Numbers*, NREL/TP-5400-61693, August 2014

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Technical Report
NREL/TP-5400-67585
February 2017

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List of Acronyms

ASTM	ASTM International
CAD	crank angle degree
CFR	Cooperative Fuel Research
CN	cetane number
CVCC	constant-volume combustion chamber
DCN	derived cetane number
FIT	Fuel Ignition Tester
HMN	2,2,4,4,6,8,8-heptamethylnonane
IQT	Ignition Quality Tester
NREL	National Renewable Energy Laboratory
PRF	primary reference fuel

Executive Summary

This report is an updated version of the 2014 *Compendium of Experimental Cetane Number Data* and presents a compilation of measured cetane numbers for pure chemical compounds. It includes all available single-compound cetane number data found in the scientific literature up until December 2016 as well as a number of previously unpublished values, most measured over the past decade at the National Renewable Energy Laboratory. This version of the compendium contains cetane values for 497 pure compounds, including 204 hydrocarbons and 293 oxygenates. One hundred seventy-five individual measurements are new to this version of the compendium, all of them collected using ASTM Method D6890, which utilizes an Ignition Quality Tester (IQT), a type of constant-volume combustion chamber. For many compounds, numerous measurements are included, often collected by different researchers using different methods. The text of this document is unchanged from the 2014 version, except for the numbers of compounds in Section 3.1; the appendices; Table 1, Primary Cetane Number Data Sources; and Table 2, Number of Measurements Included in Compendium.

Cetane number is a relative ranking of a fuel's autoignition characteristics for use in compression ignition engines. It is based on the amount of time between fuel injection and ignition, also known as ignition delay. The cetane number is typically measured either in a single-cylinder engine or a constant-volume combustion chamber. Values in the 2004 compendium derived from octane numbers have been removed and replaced with a brief analysis of the correlation between cetane numbers and octane numbers. The discussion on the accuracy and precision of the most commonly used methods for measuring cetane number has been expanded, and the data have been annotated extensively to provide additional information that will help the reader judge the relative reliability of individual results.

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1 Introduction

Cetane number (CN) is a relative measure of the time delay between the injection of fuel into the chamber and the start of combustion. Fuels for compression ignition engines must autoignite readily. If ignition does not occur promptly when the fuel is injected into the cylinder, premixed fuel and air accumulate such that when ignition does occur, the rate of burning is too rapid. The rapid burning produces high pressure rise rates that can result in engine knock that decreases efficiency and can damage the engine. Thus, the ability to rate the ignition quality of compression ignition fuels is important to diesel fuel formulation. Without adequate fuel ignition quality (a high enough cetane number), the engine will start with difficulty and run poorly.

This report presents the results of an exhaustive literature search for available experimental cetane number data for pure compounds as of December 2016 and briefly describes the process of compression ignition, the methods for measuring diesel fuel ignition quality, and the sources of uncertainty in cetane number data.

The authors anticipate that a revised and updated version of this report will be prepared every few years. Researchers are encouraged to share additional cetane number data on pure compounds as they are published for inclusion in future editions.

A compression ignition engine uses the heat of compression to ignite the fuel in the cylinders of the engine. Each cylinder is filled with air through the intake valve. The intake valve is then shut, and the motion of the piston reduces the volume of air, compressing and heating the air. At roughly the point of maximum compression, liquid fuel is injected into the cylinder through a nozzle. The fuel forms a spray of droplets that vaporize, mix with hot air, and then ignite. As the fuel burns, the gas in the cylinder heats and expands, driving the piston.

Combustion occurs in the gas phase. Thus, for a liquid fuel, the first steps toward ignition involve transitioning from a liquid to a gas. The time required for this transition is the "physical delay" in ignition and includes the amount of time required for a droplet of fuel to heat, vaporize, and mix with hot air in the cylinder.

The physical delay is influenced by [1, 2]:

- Density and temperature of the air in the cylinder
- Velocity and turbulence of the air
- Atomization, penetration, and shape of the spray
- The properties of the fuel, including:
    - Density
    - Viscosity
    - Surface tension
    - Specific heat
    - Enthalpy of vaporization

- Vapor pressure
- Vapor diffusivity.

Following the physical processes of vaporization and air mixing, a sequence of chemical reactions occurs in which the gas-phase fuel reacts with oxygen. In order to ignite, the fuel must be heated to a temperature sufficient for some of the weaker bonds within the molecules to break and form radicals. The finite rate of these radical-forming oxidation reactions is responsible for the chemical delay in compression ignition. Once a sufficient concentration of free radicals is reached, rapid oxidation occurs (ignition).

Early work by Yu et al. [3] and more recent work focused on the IQT by Bogin and coworkers [4] were able to separate the effects of physical and chemical ignition delay. While large gradients in stoichiometry and temperature occur within the IQT at DCN conditions, the chemical ignition delay is a dominant factor over the physical ignition delay for determining the measured ignition delay time and correlated DCN measurement.

2 Measuring Cetane Number

The earliest evaluations of diesel fuels were most likely audible; some fuels caused the engine to operate more smoothly than others. In time, quantitative scales were developed to more readily compare fuels.

2.1 Reference Fuels

During the 1930s, Boerlage and Broeze [5] of the Delft Laboratory in the Netherlands sought a procedure to determine the ignition quality of diesel fuel that was similar to the octane rating method for gasoline using two reference hydrocarbon fuels: 1-hexadecene and α-methylnaphthalene. The first reference fuel, 1-hexadecene, also known as cetene or ketene, has a long, straight chain structure, as shown in Figure 1, and oxidizes relatively easily. This fuel was assigned a cetene (ketene) number of 100.

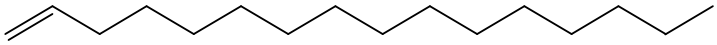

Figure 1. Structure of 1-hexadecene (cetene or ketene)

The second reference fuel, α-methylnaphthalene, also known as 1-methylnaphthalene, has two aromatic rings, as shown in Figure 2, and is highly resistant to autoignition. This fuel was assigned a cetene number of 0. The cetene number of a fuel was deemed to be the percent (by mass) of cetene in a blend of cetene and α-methylnaphthalene that gave the same ignition performance as the fuel under test.

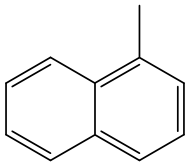

Figure 2. Structure of α-methylnaphthalene

Researchers in the United States found it was difficult to ensure all of the 1-hexadecene (cetene) had the double bond in the same position. Moreover, 1-hexadecene was prone to oxidation during storage. Because of the difficulty of preparing pure cetene, n-hexadecane (cetane) replaced cetene as the primary reference fuel (PRF) and was assigned a cetane rating of 100. The cetane number of a PRF blend was defined as:

$$\text{CN} = \%\text{ by volume n-hexadecane} + \%\text{ by volume } \alpha\text{-methylnaphthalene}$$

The structure of n-hexadecane (cetane) is shown in Figure 3.

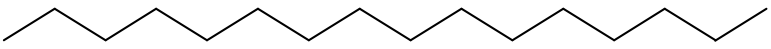

Figure 3. Structure of n-hexadecane (cetane)

Comparison of the two ratings showed the following approximate relationship between cetane rating and cetene (ketene) rating [6]:

$$\text{Cetane Rating} = 0.875 \times \text{Cetene Rating} \qquad \text{(Eq. 1)}$$

Because of experimental difficulties in working with α-methylnaphthalene, a suspected carcinogen with a foul odor, the reference fuel for the lower end of the cetane number scale was also changed. In this case the new reference fuel was 2,2,4,4,6,8,8-heptamethylnonane (HMN), shown in Figure 4, with an assigned cetane number of 15.

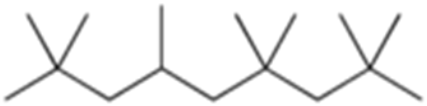

Figure 4. Structure of 2,2,4,4,6,8,8-heptamethylnonane

The ASTM International (ASTM) method for measuring cetane number is D613, Standard Test Method of Diesel Fuel Oil. The method was first published in 1941, and subsequently a key change was made, substituting HMN (CN = 15) for α-methylnaphthalene (CN = 0) as the PRF at the lower end of the scale.

The cetane number of a PRF blend is now defined as:

$$CN = \%\text{ by volume n-hexadecane} + 0.15 \times (\%\text{ by volume HMN}) \qquad \text{(Eq. 2)}$$

2.2 Test Engine Configuration

Originally, the cetene rating scale called for finding the lowest compression ratio that would produce autoignition. This proved to be imprecise. Subsequently, Boerlage and Broeze [5] proposed a method using a single-cylinder diesel Cooperative Fuel Research (CFR) engine made by Waukesha. Testing was done by injecting the fuel 10 crank angle degrees (CAD) before top dead center and adjusting a plunger in the prechamber to obtain ignition at 1 CAD after top dead center, for an ignition delay of 11 CAD. This method formed the basis for developing the ASTM D613 standard for cetane number, although the final method included a modified standard ignition delay of 13 CAD.

In the ASTM D613 test, the cetane number of a diesel fuel is determined by comparing its ignition delay in the standard CFR test engine with those for blends of reference fuels of known cetane number. The compression ratio is varied by adjusting a calibrated hand wheel to obtain the same ignition delay for the sample and for each of two bracketing reference fuels, permitting interpolation of cetane number in terms of the hand wheel readings. The ISO 5165 method, the international counterpart to ASTM D613, is essentially the same test using the same engine.

In Europe, a similar method, DIN 51773, uses a standard BASF engine for determining cetane number. Both the CFR and BASF methods vary effective compression ratios, thus varying the available energy to start combustion, but in different ways. The Waukesha CFR engine varies the physical volume of the combustion chamber, thereby changing the compression ratio of the engine and changing the amount of energy available for initiating combustion. The BASF engine, however, varies the amount of air allowed to enter the cylinder while maintaining the same physical compression ratio.

2.3 Constant-Volume Combustion Chamber

The first attempts at quantitatively measuring compression ignition fuel quality involved the use of a bench-top apparatus. Falk began to measure the compression autoignition temperature of

fuels in 1906 [7]; however, Falk did not measure the variation of cylinder pressure with time and so did not notice any ignition delay. Later, in 1914, Dixon and Howard [8] recognized the existence of an ignition delay period.

Mullins [9] reports that in 1932, Helmore and Code-Holland developed a constant-volume apparatus specifically for testing diesel fuels. The apparatus was claimed to simulate diesel engine conditions, but it operated at atmospheric pressure and could only measure ignition delays longer than 200 milliseconds. Nonetheless, they observed some agreement with the behavior of test fuels in a diesel engine.

Work by Hurn and Hughes [10] of the U.S. Bureau of Mines led to the development of a constant-volume diesel fuel test apparatus consisting of a pressurized and heated reaction chamber with a single-shot fuel injector, along with instrumentation to measure the time delay between injection and ignition. With this apparatus, the effect of cetane number on ignition delay was observed, but the researchers did not develop a specific cetane number correlation.

More recently, studies of constant-volume combustion were undertaken by Ryan and coworkers at Southwest Research Institute with the goal of developing a new method for rating the ignition delay of diesel fuels [11, 12]. These studies resulted in the development of an ignition quality tester (IQT) in which a sample of fuel is injected into a heated, constant-volume combustion chamber (CVCC). Initially the pressure decreases due to cooling from fuel evaporation, but rises as combustion begins reaching the initial pressure at the pressure recovery point. The ignition delay is measured as the time delay between the beginning of injector needle lift and the chamber pressure recovery point. A correlation was developed between the observed ignition delay and the cetane number. The method has been refined, validated, and commercialized by Advanced Engine Technology, Ltd. [13, 14, 15] and has been approved by ASTM as Standard D6890. A similar method using the Waukesha Fuel Ignition Tester (FIT) has been formalized in ASTM Standard D7170. Most recently, Herzog by PAC has introduced the Cetane ID 510 with associated ASTM Standard D7668. Prior to finalization of these ASTM standards, cetane numbers were obtained using similar equipment (in some cases these CVCC prototypes), although the methodology may not have met all of the requirements of the ASTM standards.

CVCC methods use much smaller sample volumes than the engine test procedure (on the order of 100 milliliters versus 1 liter for the engine test), which can be significant for expensive and difficult-to-produce pure compounds. The CVCC methods can also be completed in much shorter time frame (20 minutes versus a few hours). Moreover, because the reproducibility errors (discussed in more detail in Section 3.5) are lower for the IQT than those found for the CFR engine, it is generally considered the better method for measuring cetane number at this time. Most new data reported in this version of the compendium are IQT values.

Because the cetane number determined by CVCC methods is not measured in the actual CFR engine, which is the defined source of cetane number values, the values that result from this approach are known as the *derived cetane number* (DCN). The CVCC methods are calibrated to the CFR engine using hydrocarbon compounds. In practice, correlation between the methods has been quite good for the mid-range cetane number distillate fuels for which both the CVCC and the CFR methods are most commonly used. However, because each method measures ignition delay under different conditions (pressure, temperature, and stoichiometry), it is possible that the

effects of these different operating conditions may not result in the same correlation for all compounds [14, 16]. For ASTM standard compliance, the D613 CFR engine method remains the referee method.

2.4 Blending Cetane Numbers

In some cases, cetane number data were not available for the pure compound, but were available for blends of a known volume of the pure compound in diesel fuel of known cetane number. In such cases, it is possible to compute a blending cetane number. However, the typical methodology for developing blending cetane numbers results in an amplification of uncertainty. Assuming the cetane number of the blend is a linear combination of the cetane numbers of the components, we expect for a 10% blend:

$$\text{Blend CN} = (0.9) \times (\text{Base Fuel CN}) + (0.1) \times (\text{Test Fuel CN}) \quad \text{(Eq. 3)}$$

or

$$\text{Test Fuel CN} = [(\text{Blend CN}) - (0.9) \times (\text{Base Fuel CN})] / 0.1 \quad \text{(Eq. 4)}$$

However, any measurement error in the blend CN will be multiplied by the inverse of the blend level when the test fuel CN is calculated (e.g., a 20% blend results in a five-fold increase in the magnitude of the error; see sample calculation in box). Inasmuch as the base fuel cetane number measurement is also subject to measurement error and that many studies report cetane number measurement errors greater than 0.5 CN, the possibility exists for large errors in the reported blending cetane numbers.

A separate issue is whether or not the cetane number of a blend is indeed a linear combination of the cetane numbers of the components. Although the CFR cetane number scale is based on the linear blending values of the two PRFs, n-hexadecane and HMN, there is evidence that the linear assumption is not correct for all blends. For example, in their study of the cetane numbers of carboxylic esters, Serdari et al. [17] find the cetane numbers of methyl oleate blends appear to behave linearly, while those of ethyl laurate blends appear to behave non-linearly. Nonetheless, blending cetane number data may be the only information available for some pure components. In the compendium of cetane numbers, blending cetane numbers are included, but are flagged to warn users of the possible uncertainties. However, for this reason, it is recommended that blend values be considered a rough approximation of the actual cetane number. If better information is available from tests of the compound in pure form the use of those values is preferred.

Example of Amplification of Measurement Error in Blend Fuel Calculations:

If the base fuel CN is 50 and the test fuel CN is 10, a 10% blend of test fuel in the base fuel, assuming CN is a linear combination of the components (using Eq. 3), the true CN value of the blend is:

$$\text{Blend CN} = (0.9) \times (50) + (0.1) \times (10) = 46$$

If the measured CN is 47, only 1 CN point larger than the true value, then, using Eq. 4, the calculated value of the test fuel CN would be:

Calculated test fuel CN = $[(47) - (0.9) \times (50)] / 0.1 = 20$, a CN value that is 10 CN points larger than the true value.

3 Cetane Number Data Quality

3.1 Origin of Data

Referenced sources and technical papers were sought in which cetane number data were presented for pure compounds. Based on this search conducted first in 2004 and then again in 2013, a summary of all available cetane number data for pure compounds was developed and is included in Appendix A. The results include the measured cetane numbers of 496 pure compounds, including 204 hydrocarbons and 292 oxygenates. The total number of measurements is 760, from 77 different sources, which include many compounds for which there are values available from more than one source, and many measurements that appear to have been cited in more than one source. Where that was apparent, those data points have been combined in the appendix. All sources for the information are cited in Appendix B.

There are several references that have been used as "handbooks" of cetane number data. One recent source of cetane number data is the 1999 book *Fuels and Engines* by J.C. Guibet [18], which lists cetane number data for approximately 100 pure compounds. However, these data are, in fact, the same cetane number values[*] for the same compounds that are found in *Technical Data on Fuels* by Rose and Cooper, published in 1977 [19].

The data in Rose and Cooper are not individually referenced, but are stated to be taken mainly from the 1948 U.S. Bureau of Mines Information Circular 7474 by Puckett and Caudle that contains cetane number data for 98 compounds [20]. The Bureau of Mines circular contains references to the source of each cetane number value. From these references we learn that cetane numbers for most of the compounds in Circular 7474 are quoted from work done by Petrov in Russia from 1938 to 1946 using a combustion bomb apparatus called the Nuemann bomb to measure ignition delay, then using a correlation between ignition delay and cetene number. A 1938 correlation between the cetene number scale and the cetane number scale, cited in Section 2.1, was applied to "convert" Petrov's results to a cetane number value. Another recent source, Chevron's *Diesel Fuels Technical Review* [21] lists cetane numbers for 21 compounds. No references are given for these data, but there are indications that they too are derived from the Russian work quoted by Puckett and Caudle.[†] Multiple identical values of the same cetane number were reduced to a single line in the appendix and attributed to all of the sources in which they appear and which we were able to obtain. Thus, the many data points attributed to any one of these sources were likely derived from World War II-era ignition delay measurements and the successive application of two correlations (from ignition delay to cetene number and from cetene number to cetane number).

Serdari et al. [16] present cetane numbers for 64 esters measured in blends of only 5% to 7%, and they estimate their precision at ±7 to 10 cetane units. Knothe, Matheaus, and Ryan [22] present cetane number data for 29 fatty acid esters. In an earlier paper, Knothe, Bagby, and Ryan [23] list cetane numbers derived from an ignition delay procedure for 21 esters, alcohols, and triglycerides. Freedman et al. [24] present data for 20 esters, alcohols, and triglycerides. There is

[*] There is a transcription error for 2-methyl-4-isobutyl-4-phenylundecane: instead of the cetane number of 18 found in Rose and Cooper, Guibet lists a cetane number for this compound of 38.

[†] A "5" for "8" transcription error for the cetane number of 3-ethyldecane that occurred going from a 1946 review paper prepared by Petrov to the Bureau of Mines report and then carried through all the later references supports this hypothesis.

substantial overlap between these sources in terms of compounds studied; where there is overlap, the agreement is often poor. Most data for fatty acid esters are from a CVCC-based ignition delay apparatus. Only a few values are reported to be from the D613 engine test, and in those cases the experimental procedure is poorly documented considering that in some cases the esters tested are solids at normal ambient temperatures. It is not clear whether the entire apparatus was heated above the melting point or whether the values reported are actual blending cetane numbers with an unspecified diesel fuel.

In the original 2004 version of the compendium, the National Renewable Energy Laboratory (NREL) was the source of 26 data points, all measured on the IQT. Additional compounds measured on the NREL IQT bring the total number of compounds measured at this laboratory to 108, including a range of alkanes, iso-alkanes, cyclo-alkanes, alkenes, aromatics, esters, alcohols, and ethers using ASTM D6890 (IQT). Some of these have been published in scientific literature, but many are published here for the first time.

This compendium also includes individual values collected in small numbers from a variety of scientific papers. Table 1 lists the most important sources of data in this compendium. These seven sources comprise approximately 70% of the data in this version of the compendium. As noted above, there is considerable overlap in the measurements listed in References 3 and 4 in Table 1.

Table 1. Primary Cetane Number Data Sources

Reference Number	Reference	Number of Measurements Included in Compendium
41	NREL IQT data	108
3	Puckett, A.D.; Caudle, B.H. (1948). *Ignition Qualities of Hydrocarbons in the Diesel Fuel Boiling Range*. Bureau Mines Information Circular 7474.	98
4	Rose, J.W.; Cooper, J.R. (1977). “Detonation of Liquid Fuels.” In *Technical Data on Fuel*.	89
76	Dahmen, M.; Marquardt, W. (2015) "A Novel Group Contribution Method for the Prediction of the Derived Cetane Number of Oxygenated Hydrocarbons." *Energy Fuels* 29 (9); pp. 5781–5801.	79
32	Serdari, A.; Lois, E.; Stournas, S. (1999). “Impact of Esters of Mono- and Dicarboxylic Acids on Diesel Fuel Quality.” *Ind. Eng. Chem. Res.* (38); p. 3543.	64
1	Olson, D.R.; Meckel, N.T.; Quillian, R.D. (1960). “Combustion Characteristics of Compression Ignition Engine Fuel Components.” SAE paper 600112.	40
33	Knothe, G.; Matheaus, A.C.; Ryan III, T.W. (2003). “Cetane Numbers of Branched and Straight-Chain Fatty Esters Determined in an Ignition Quality Tester.” *Fuel* (82); p. 971.	28

3.2 Purity of Compounds

There are few data on the purity of the compounds that were used for cetane number determinations. Because of the relatively large sample size required for the ASTM D613 engine test, assembling samples of high purity levels is challenging and potentially very expensive. Older data typically did not include information on purity levels or the identity of possible impurities.

Peroxides (compounds with an R-O-O-R linkage), in particular, have been found in many compounds at levels sufficient to affect the measured cetane number [25]. Because most peroxides are extremely reactive, they have long been known to be effective additives for improving the cetane number of diesel fuels [26]. Peroxides can be formed by the auto-oxidation of hydrocarbons in storage. Even the n-hexadecane (cetane) diesel reference fuel can contain peroxides that affect the results of cetane number determinations.

ASTM D6890 requires all samples be filtered through a 3–5-micron filter to remove particulates and that the sample be at room temperature (18°C–32°C). However, because calibrating the IQT with the low cetane check fuel (methylcyclohexane) was so frequently problematic, Advanced Engine Technology (the owner of the IQT technology) investigated sample purity to determine the source of the contamination [27].The study found that filtering methylcyclohexane through a (250°C treated) silica gel column improved the ignition delay reproducibility. Although specific contaminants were not identified in this study, silica gel is polar and will adsorb and remove polar contaminants like water or oxygenates. To ensure high purity and the removal of peroxides, modern standard practice for hydrocarbons and non-polar oxygenates employs column chromatography on samples prior to testing. All samples should be evaluated for their purity prior to testing.

3.3 Reference Compounds

The accuracy of the definition of HMN as a PRF with a cetane number of 15 was called into question as long ago as the 1974 study by Bowden et al. of Southwest Research Institute [28]. He reported that, using α-methylnaphthalene and hexadecane as reference fuels, the cetane number of HMN was found to be only 12.2 and not 15, as is customarily assigned when it is used as a reference fuel. IQT measurements of HMN at NREL produce a consistent DCN value of 15.1.

For fuels with cetane numbers typical of diesel fuels in the United States (in the low 40s), this would make a difference of slightly more than one cetane number unit when comparing data from cetane number scales based on the older and newer reference compounds.

3.4 Low and High Cetane Number Fuels

Currently there is no accepted methodology for extending the cetane number scale to cetane numbers less than zero or greater than 100. While this can be done using blending cetane numbers, this approach is not rigorous and in some cases leads to very different results with different base fuels. Many samples tested using the IQT included in this compendium fall outside the limits of ASTM D6890 (33 to 64 DCN). Testing has not been undertaken to ensure repeatability and reproducibility of samples outside this range, nor have comparisons been conducted to ensure that the DCNs correspond to CN as measured by D613.

3.5 Accuracy of Cetane Number Determinations

Table 2 lists the number of data points included in this compendium from each type of measurement method. Upon review of the original sources, a number of measurements have been reclassified from the original compendium. These changes have been included in the notes in Appendix A.

Blend measurements, by their nature, are less accurate than the underlying measurement method. Unknown methods and other ignition delay methods suffer from varying methodology and uncertain correlation, as well as generally being older and thus potentially made using samples of lesser purity. Thus, data collected using ASTM D613 (CFR), D6890 (IQT), and D7170 (FIT) should be considered the most trustworthy because the methods themselves are well documented, consistently implemented, and correlated with each other.

Table 2. Number of Measurements Included in Compendium

	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Total
Measurements in 2004 Compendium	3	16	0	76	85	142	322 measurements, 296 different compounds
Measurements in 2014 Compendium	58	128	6	70	135	189	586 measurements, 387 different compounds
Measurements in this Compendium	58	303	6	70	135	189	761 measurements, 497 different compounds

In instances where cetane number data are available from more than one source, there is often poor agreement as shown in the graph below; differences of up to 15 cetane numbers are not uncommon in this compendium. The current ASTM methods D613, D6890, and D7170 (the CFR engine, IQT, and FIT procedures, respectively) list reproducibility and repeatability limits for the accepted range of the specification. Those values are shown in Figures 5 and 6. ASTM defines reproducibility as the difference between two test results on identical samples, but obtained by different operators in different laboratories, that would be exceeded only one case in 20. In other words, for D613 tests on a cetane number 48 fuel by multiple laboratories, 95% of the test results would be between 44.2 and 51.8. Repeatability is the difference between two test results on identical samples obtained by the same operator using the same apparatus, under constant operation conditions, on identical test materials that would be exceeded only one time in 20.

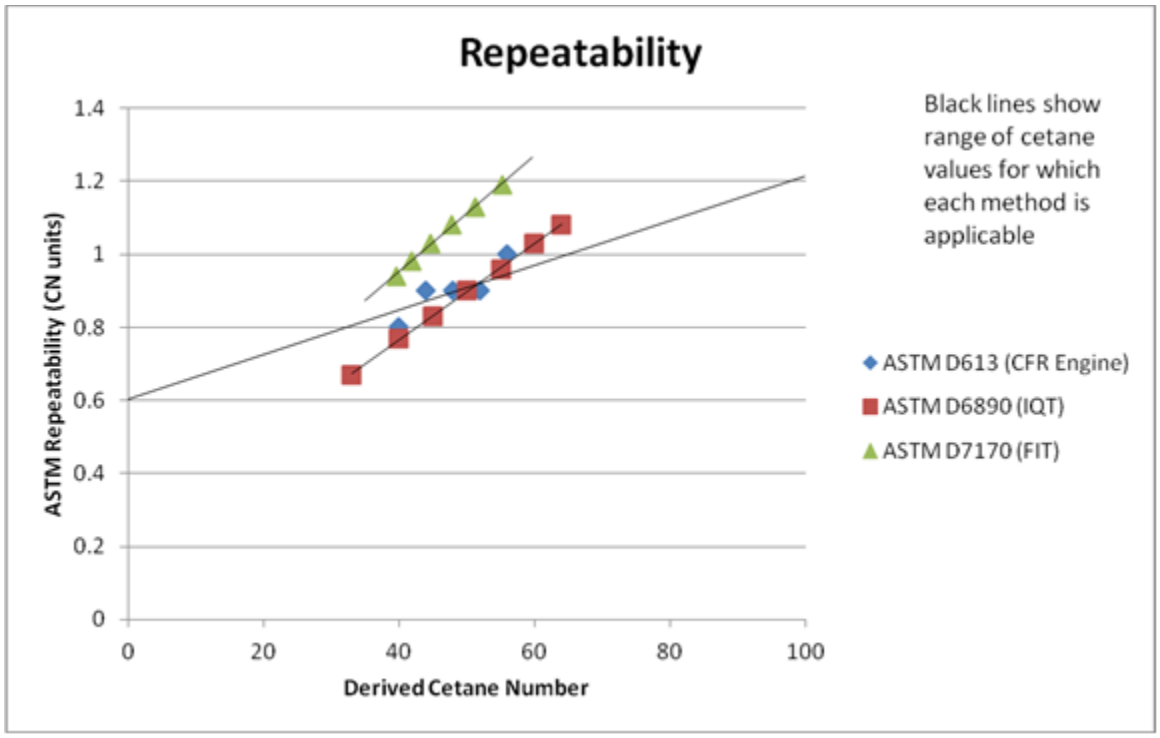

Figure 5. ASTM repeatability of ASTM D613, ASTM D6890, and ASTM D7170

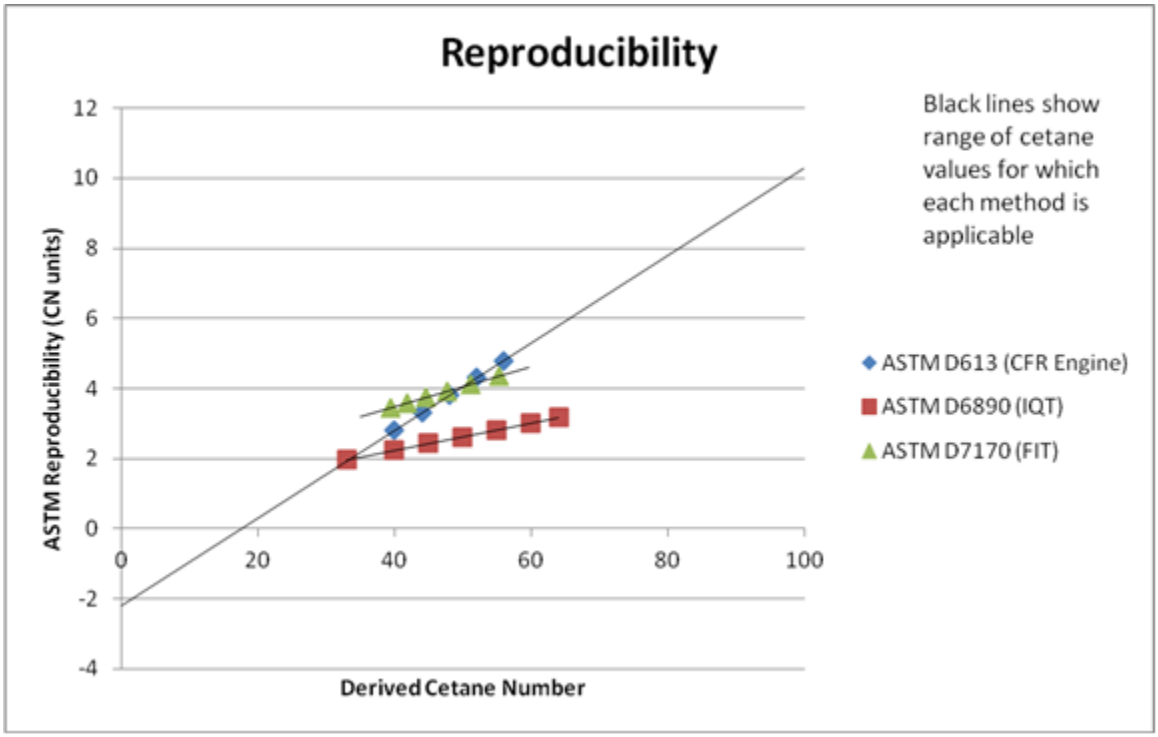

Figure 6. ASTM reproducibility of ASTM D613, ASTM D6890, and ASTM D7170

These graphs show that within the tested range, the IQT method has the best reproducibility of the three methods and its repeatability is comparable to that of the CFR engine approach. In fact, in this compendium, for the 18 compounds that were measured more than once by IQT, generally in different laboratories with different samples, the standard deviation averaged approximately 3 cetane units, comparable to the reproducibility shown in Figure 6. The FIT method has a lower repeatability than the other two methods, and its reproducibility is comparable to that of the CFR engine approach.

It is well known that the correlation between results from ASTM D613 and D6890 is not perfect for many compounds [14, 16] because the methodologies used are not testing exactly the same fuel characteristic. Similarly, it should be expected that the correlation between ASTM D613 and ASTM D7170 (the FIT method) may not correlate exactly for the same reason. Figure 7 shows how measurements made using various approaches compare to the same compound measured in the ASTM D613 CFR engine. Because these tests were done by different laboratories on different samples, some of the variation is likely due to sample impurities. Table 3 shows the average absolute difference in DCN as measured by IQT and other methods.

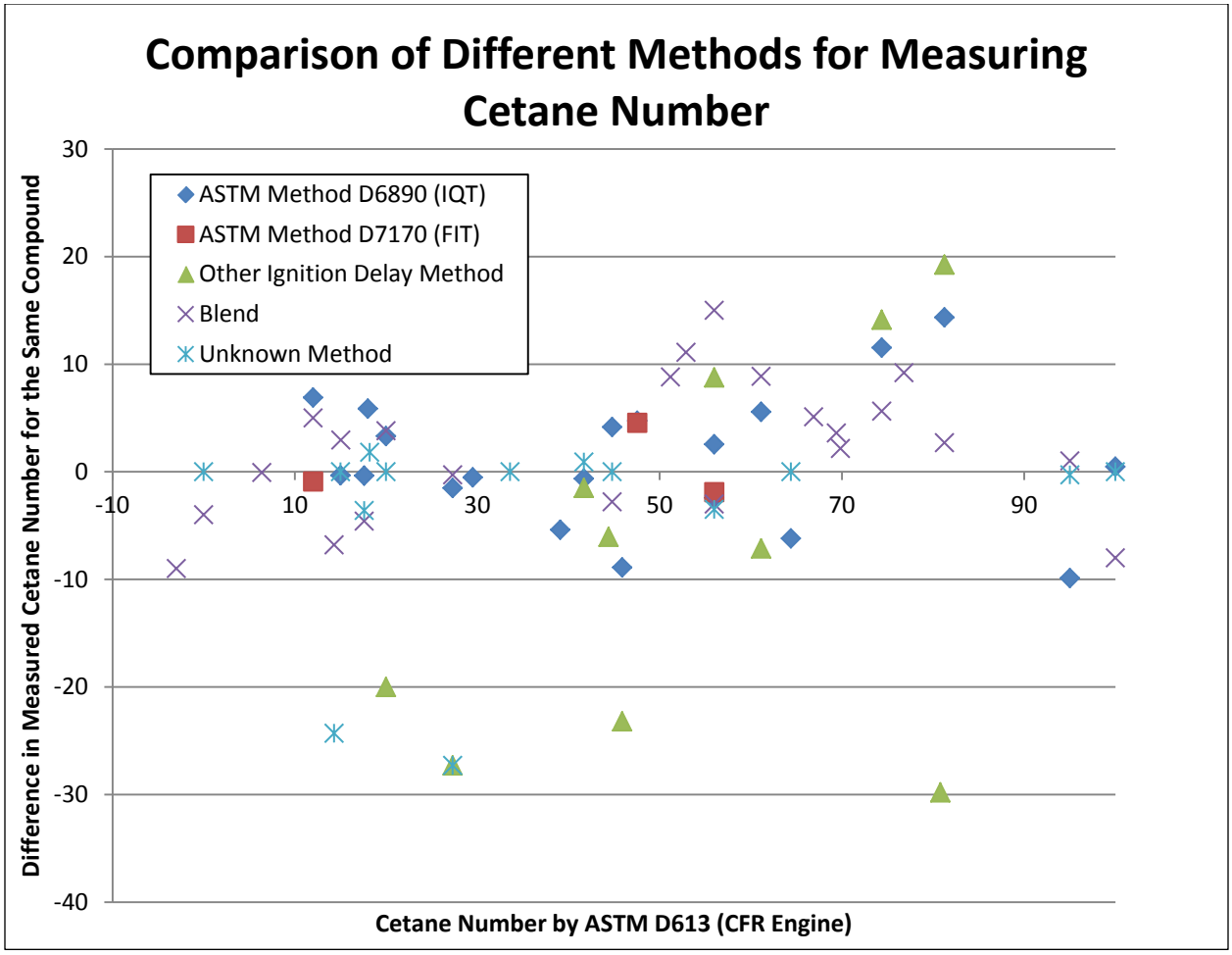

Figure 7. Comparison of different methods for measuring cetane number

Table 3. Average Absolute Difference between DCN by IQT and Values Measured by Other Methods

Method	ASTM Method D613 (CFR)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method
Average Difference	4.8 (20 compounds)	2.5 (3 compounds)	15.7 (10 compounds)	5.4 (23 compounds)	4.4 (14 compounds)

Note: The last update to this table was in the 2014 Compendium.

3.6 Estimation Methods for Cetane Number

In 1995, Ladommatos [29] and coworkers reviewed numerous methods used to correlate the cetane number with various physical and chemical attributes of a blend or individual compounds in the fuel, but model predictions of cetane number continue to be a fruitful area of research [30, 31, and many more]. These include correlations based on properties such as density, boiling points, and molecular composition. While a thorough review is beyond the scope of this document, Figure 8 shows the correlation between research octane number (RON), as determined using ASTM D2699, and cetane number using all readily available data (cetane number from this compendium and octane numbers from two comprehensive sources [32, 33]). In addition, an earlier correlation, developed by Bowden and coworkers, is included in the graph over the range of values that was considered in their work [27]. In the 2004 compendium, some values of cetane number derived from a correlation with octane number were included in the cetane number tables. In this document, use of the correlation is left to the reader, and only experimentally measured cetane numbers are included in Appendix A.

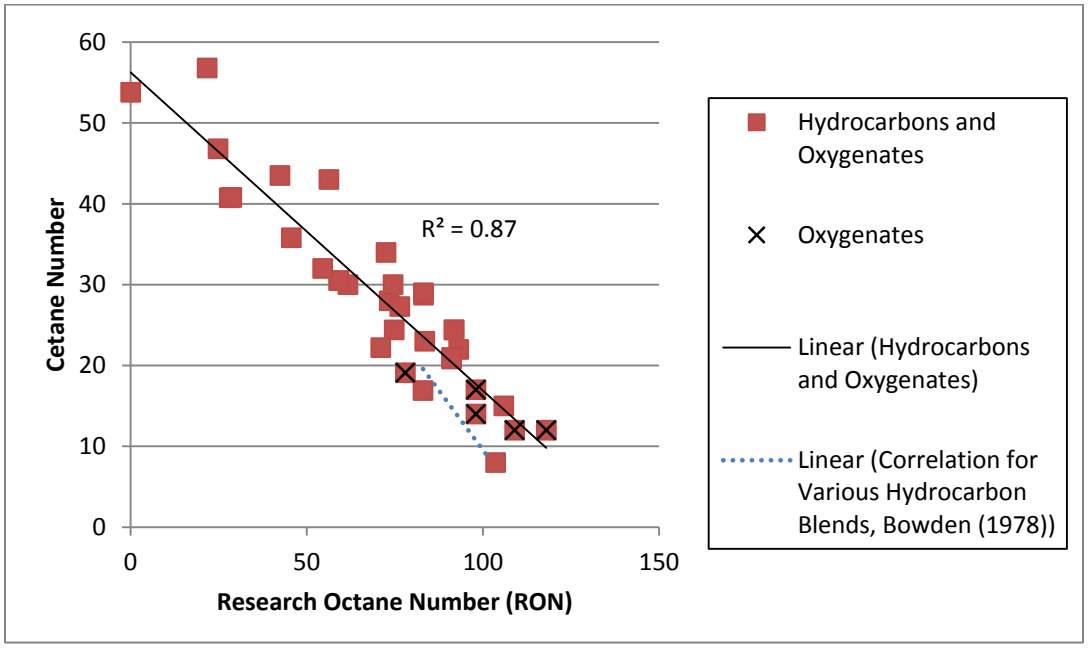

Figure 8. Correlation between cetane number and research octane number suggests cetane number for both oxygenates and hydrocarbons can be roughly estimated as 56 – (0.39 x research octane number).

4 Summary

All available experimental cetane number data for individual compounds are included in Appendix A. The listing is organized by compound class and then by molecular formula. The method used to derive the value is noted. Data from empirical cetane number correlations are not included in this compendium, with the exception that early data converted from cetene numbers are included where noted in the Comments column.

Based on this survey, we find:

- A total of 761 measurements of cetane number are reported for a total of 497 compounds.
- In many cases, duplicate data for the same compound do not agree.
- ASTM D6890 and ASTM D7170 are limited by testing that has only investigated accuracy and precision over a very narrow range of DCNs representative of typical diesel fuels.
- Nonetheless, the data collected using ASTM D613, D6890, or D7170 during the past decade represent the most accurate information available. Those data are in the green columns in Appendix A.
- Recent results have demonstrated that the presence of peroxide impurities can make a substantial difference in the measured cetane number.
- The purity of many of these compounds is unknown or is suspect.
- There is no accepted extension of the cetane number scale beyond 0 or 100 despite the need to characterize compounds with lower and higher cetane numbers.

Appendix A. Compendium of Experimental Cetane Number Data

A.1 Alkanes

A.1.1 n-Alkanes

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
n-propane	C3H8	74-98-6						-20	37	
n-butane	C4H10	106-97-8		20.6					77	new
n-pentane	C5H12	109-66-0					30		1	[1], [30]
n-hexane	C6H14	110-54-3	44.8						9	
				47.9					41	[2]
				50.0					49	
							42		1	[1], [30]
								45	2	
n-heptane	C7H16	142-82-5	56.0						3,4	[27]
				53.8					41	[2]
				53.0					49	
				53.7					51	
				53.8					59	[4]
					54.1				65	
							53		1	[1], [30]
				53.8					72	new
				53.8					77	new
				52.8					76	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
n-octane	C8H18	111-65-9	64.4						9	[35]
				58.2					41	[2]
								65	2	
								64	5	[22]
n-nonane	C9H20	111-84-2		60.9					41	
							74		1	[1], [30]
								72	2,6	
n-decane	C10H22	124-18-5		65.5					41	
				67.2					64	
							65		62,63	[6], [32]
								78	2	
								76	4	
								77	5	[22]
								76	7	
n-undecane	C11H24	1120-21-4					79		1	[1], [30]
								83	2,6	
n-dodecane	C12H26	112-40-3		72.9					41	
				74.0					49	
							78		61,63	[6],[33]
								88	5	[22]
								80	3,4	
n-tridecane	C13H28	629-50-5						88	4	
								91	2,6	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
n-tetradecane	C14H30	629-59-4	95.0						9	[35]
				85.1					41	
							96		1	[1], [30], [35]
								95	2	
								93	4	
								96	5	[22]
n-pentadecane	C15H32	629-62-9						98	2,6	
								95	4,7	
n-hexadecane	C16H34	544-76-3	100.0						PRF	[9]
				100.5					41	
							92		1	[1], [30]
								100	4	
				98.5					76	new
n-heptadecane	C17H36	629-78-7						105	4	
n-octadecane	C18H38	593-45-3						110	4	[5]
								103	5	[5],[22]
n-nonadecane	C19H40	629-92-5						110	4	[5]
n-eicosane	C20H42	12-95-8						110	4, 7	[5]

A.1.2 iso-Alkanes

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2-methylbutane	C5H12	78-78-4		24.0					76	new
				25.8					77	new
2,2-dimethylbutane	C6H14	75-83-2		24.4					41	
2-methylpentane	C6H14	107-83-5					29		1	[1], [23], [30]
								33	4	
				34.5					41	
3-methylpentane	C6H14	96-14-0	30.0						3,4	[27]
				30.7					77	new
2,2,3-trimethylbutane	C7H16	464-06-2		12.9					41	
2,3-dimethylpentane	C7H16	565-59-3		22.0					41	
				21.7					77	new
2,4-dimethylpentane	C7H16	108-08-7					29		1	[1], [30], [35]
				28.7					41	
				28.2					77	new
2-methylhexane	C7H16	591-76-4		43.5					41	
3-ethylpentane	C7H16	617-78-7		34.1					41	
3-methylhexane	C7H16	589-34-4		42.0					77	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2,2,4-trimethylpentane	C8H18	540-84-1	17.6						9	[35]
			12.0						3,4	[27]
				17.2					41	
				18.9					58	
					11.1				65	
							17		62,63	[6],[32]
							13		1	[25],[30],[37]
								14	6	
				17.4					77	new
2-methylheptane	C8H18	592-27-8		52.6					41	
				47.0					54	
2,2,5-trimethylhexane	C9H20	3522-94-9					24		1	[1], [30],[37]
								24	1,8	
2,2-dimethyloctane	C10H22	15869-87-1						59	7	
2,6-dimethyloctane	C10H22	2051-30-1		51.7					41	[7]
2,2,4,6,6-pentamethylheptane	C12H26	13475-82-6						9	3	[8]
								9	4,11	
3-ethyldecane	C12H26							48	3	[8], [23]
								48	7,10	
4,5-diethyloctane	C12H26	1636-41-5						20	3	[8]
								20	7	
2,5-dimethylundecane	C13H28	17301-22-3						58	3	[8]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
4-propyldecane	C13H28							39	3,4	[8]
5-butylnonane	C13H28	17312-63-9						53	3,4	[8]
2,7-dimethyl-4,5-diethyloctane	C14H30							39	3,4	[8]
farnesane (2,6,10-trimethyldodecane)	C15H32	3891-98-3		58.0					50	
				59.1					60	
2,2,4,4,6,8,8-heptamethylnonane	C16H34	4390-04-9	15.0						PRF	[9]
				15.1					41	
				14.2					64	
								15	7	
				14.2					76	new
5-butyldodecane	C16H34	6118-01-0						45	4	
7,8-dimethyltetradecane	C16H34	2801-86-7						40	3,4	[8]
7-butyltridecane	C17H36							70	3,4	[8]
2-methylheptadecane	C18H38	18869-72-2		91.0					41	
5,6-dibutyldecane	C18H38							30	3,4	[8]
7,8-diethyltetradecane	C18H38	500020-70-2						67	3	[8]
								67	4,11	
8-propylpentadecane	C18H38							48	3	[8]
								48	4,7	
9-methylheptadecane	C18H38	18869-72-2						66	3,4	[8]
2-methyloctadecane	C19H40	1560-88-9		104.4					41	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
9,10-dimethyloctadecane	C20H42							60	3,4	[8]
7-hexylpentadecane	C21H44							83	3,4	[8]
2,9-dimethyl-5,6-diisopentyldecane	C22H46							48	3,4	[8]
10,13-dimethyldocosane	C24H50							56	11	
9,10-dipropyloctadecane	C24H50							47	3,4	[8]
9-heptylheptadecane	C24H50							88	3,4	[8]

A.1.3 Cycloalkanes

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
cyclopentane	C5H10	287-92-3		6.1					41	
cyclohexane	C6H12	110-82-7	16.9						9	[35]
			13.2						3,4,6	[27]
							18		1	[1], [30]
				19.9					77	new
				20.0					76	new
methylcyclopentane	C6H12	96-37-7		17.2					41	
methylcyclohexane	C7H14	108-87-2	20.0						3,4	[27]
				24.4					41	[7]
				22.0					55	
				23.5					59	[4]
							24		1	[1], [30], [37]
								20	5	[22]
1,2-dimethylcyclohexane	C8H16	583-57-3		24.0					77	new
1,3-dimethylcyclohexane	C8H16	591-21-9		30.5					77	new
cyclooctane	C8H16	292-64-8		22.3					41	
ethylcyclohexane	C8H16	1678-91-7		35.8					41	
1,2,4-trimethylcyclohexane	C9H18	2234-75-5		24.4					76	new
1,3,5-trimethylcyclohexane	C9H18	1839-63-0		30.5					41, 54	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
tetrahydro-dicyclopentadiene	C10H16	2825-82-3		20.4					74	new
cis-decalin	C10H18	91-17-8		39.4					41	[2]
				41.6					55	
decalin	C10H18	91-17-8						48	3	[8],[36]
								42	5	[22]
								48	4,7	[36]
trans-decalin	C10H18	91-17-8		31.8					41	
				32.0					55	
n-butylcyclohexane	C10H20	1678-93-9		47.6					41	
				48.0					54	[3] old value was 46.5
2-ethyladamantane	C12H20			42.7					75	new
bicyclohexyl	C12H22	92-51-3						47	5	[22]
								53	3,4	
3-cyclohexylhexane	C12H24							36	3	[8]
								36	4,7	
propyladamantane	C13H22			48.6					75	new
n-propyldecalin	C13H24							35	3,4	[8]
butyladamantane	C14H24	14449-41-3		49.1					75	new
perhydrophenanthrene	C14H24	5743-97-5		38.8					41	[7]
n-butyldecalin	C14H26							31	3,4	[8]
sec-butyldecalin	C14H26							34	3,4	[8]
tert-butyldecalin	C14H26							24	3,4	[8]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
pentyladamantane	C15H26			48.5					75	new
1,3,5-triisopropylcyclohexane	C15H30	34387-60-5		25.3					41	
2-methyl-3-cyclohexylnonane	C16H32							56	3	[8]
								70	7	
n-octyldecalin	C18H34							31	3,4	[8]
1-methyl-3-dodecylcyclohexane	C19H38							70	3,4	[8]
2-cyclohexyltetradecane	C20H40							57	7	
								57	3,4	[8]
2-methyl-2-cyclohexylpentadecane	C22H44							45	3,4	[8]
1,2,4-trimethyl-5-hexadecylcyclohexane	C25H50							42	3,4	[8]
5-cyclohexyleicosane	C26H52							66	3,4	[8]

A.2 Alkenes

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2-methyl-1,3-butadiene	C5H8	78-79-5		13.0					76	new
Cyclohexene	C6H10	110-83-8					57		1	[1], [30], [37]
				18.1					76	new
1-hexene	C6H12	592-41-6	27.3						9	[35]
				25.8					41	
							27		1	[1], [30]
				28.9					77	new
1-heptyne	C7H12	628-71-7		22.0					41	
4-methyl-1-cyclohexene	C7H12	591-47-9					52		1	[1], [30]
1-heptene	C7H14	592-76-7		32.0					41	
cis-2-heptene	C7H14	14686-13-6					44		1	[1],[10], [30]
1,5-cyclooctadiene	C8H12	111-78-4		25.7					76	new
4-vinyl-1-cyclohexene	C8H12	100-40-3					40		1	[1], [30]
2,5-dimethyl-2,4-hexadiene	C8H14	764-13-6		19.9					76	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1-octene	C8H16	111-66-0		40.0					41	
								41	2,6	
								41	5	[22]
2,4,4-trimethyl-1-pentene	C8H16	107-39-1					11		1	[1], [30]
								10	4	
				8.8					77	new
							-3		1	[1], [30], [37]
2-octene	C8H16	111-67-1					43		1	[1], [30]
cis-3-octene	C8H16	14850-22-7		38.1					48	
trans-3-octene	C8H16	14919-01-8		34.0					48	
1-nonene	C9H18	124-11-8						51	2,6	
2,4-dimethyl-2-heptene	C9H18	860116-58-1		27.0					73	new
2,6-dimethylheptene	C9H20	1072-05-5					51		1	[1], [30]
(R)-(+)-limonene	C10H16	5989-27-5		19.0					73	new
3-carene	C10H16	13466-78-9		27.0					41	new
limonene	C10H16	138-86-3		18.9					76	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
ocimene	C10H16	13877-91-3		28.0					41	new
α-pinene	C10H16	80-56-8		18.9					76	new
				23.5					41	[7]
				27.0					73	new
β-pinene	C10H16	127-91-3		20.5					76	new
				22.0					41	[7]
γ-terpinene	C10H16	99-85-4		20.3					76	new
1,9-decadiene	C10H18	1647-16-1		41.0					41	[2]
1-decene	C10H20	872-05-9		49.1					41	
								60	2	
								60	5	[22],[23]
								59	2,6	
1-undecene	C11H22	821-95-4						66	2	
								65	2,6	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1-dodecene	C12H24	112-41-4		56.8					41	
								71	2,6	
								71	5	[22]
1-tetradecene	C14H28	1120-36-1						83	5	[22]
								81	2,6	
								79	3,4	[8]
bisabolene	C15 H24			32.2					41	[7]
caryophyllene	C15H24	87-44-5		29.0					41	new
farnesene	C15H24	502-61-4		32.0					41	new
2,6,7-trimethyl-2,6-tridecadiene	C16H30							24	3,4	[8]
1-hexadecene	C16H32	629-73-2		75.9					41	
								86	2,6	
								88	3	
								84	5	[22]
2,2,6,6,8,8-hexamethyl-4-methylene-nonane	C16H32	15220-85-6						5	3	
4-butyl-4-dodecene	C16H32							45	11	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
5-butyl-4-dodecene	C16H32							45	3,4	[8]
7-butyltridecene	C17H34							36	3,4	[8]
3,12-diethyl-3,11-tetradecadiene	C18H34							26	3,4	[8]
1-octadecene	C18H36	112-88-9						90	5	[22]
7,10-dimethyl-8-hexadecene	C18H36							43	3,4	[8]
8-propyl-8-pentadecene	C18H36							45	3,4	[8]
9-methyl-9-heptadecene	C18H36							66	3,4	[8]
7-hexyl-7-pentadecene	C21H42							47	3,4	[8]
10,13-dimethyl-11-doeicosene	C24H48							56	3,4	[8]

A.3 Aromatics

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
benzene	C6H6	71-43-2	14.3						9	[35]
							15		1	[1],[23], [30]
							0		3	
								-10	3,6	[11]
toluene	C7H8	108-88-3					3		1	[1], [23], [30]
							-5		3	
							0		58	[6],[34]
				6.0					77	new
1,2-dimethylbenzene	C8H10	95-47-6	8.3						9	[35]
				8.3					77	new
1,3-dimethylbenzene	C8H10	108-38-3					-1		1	[1],[23], [30]
				7.0					77	new
1,4-dimethylbenzene	C8H10	106-42-3					-4		1	[1],[23], [30]
				6.2					77	new
ethyl benzene	C8H10	100-41-4					4		1	[1],[23], [30]
				6.3					77	new
indan	C9H10	496-11-7		8.6					77	new
1,2,3-trimethylbenzene	C9H12	526-73-8		10.1					77	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1,2,4-trimethylbenzene	C9H12	95-63-6		8.9					41	
				8.9					77	new
1,3,5-trimethylbenzene	C9H12	108-67-8					8		63	[6],[28]
				8.0					77	new
isopropyl benzene	C9H12	98-98-8					7		1	[1],[23], [30]
n-propylbenzene	C9H12	103-65-1					16		63	[6],[28]
benzaldehyde dimethyl acetal	C9H12O2	1125-88-8		10.4					76	new
α-methyl-trans-cinnamaldehyde	C9H8O	14371-10-9		19.1					76	new
tetralin	C10H12	119-64-2		8.9					41	
				21.3					55	
							15		1	[1],[23], [30]
				9.4					77	new
1,2,4,5-tetramethylbenzene	C10H14	488-23-3					1		1	[1],[23], [30]
1,3-diethylbenzene	C10H14	141-93-5					5		1	[1],[23], [30]
1-methyl-4-isopropylbenzene	C10H14	99-87-8					4		1	[1],[23], [30]
n-butylbenzene	C10H14	104-51-8		12.0					41	
				12.9					76	new
sec-butylbenzene	C10H14	135-98-8					6		1	[1],[23], [30]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
tert-butyl benzene	C10H14	98-06-8					0		1	[1],[23], [30]
naphthalene	C10H8O	91-20-3					22		1	[26],[30], [37]
1-methylnaphthalene	C11H10	90-12-0	0.0						PRF	[9]
							-4		1	[1],[23], [30]
								0	3,6,7	
2-methylnaphthalene	C11H10	91-57-6					6		1	[1], [30], [37]
n-pentylbenzene	C11H16	538-68-1					18		3	[35]
								9	3	[8]
								8	7	
biphenyl	C12H10	92-52-4					12		1	[26],[30], [37]
							21		3	[35]
								21	7	
2,6-dimethylnaphthalene	C12H12	581-42-0					-7		1	[1],[23], [30]
1,3,5-triethylbenzene	C12H18	102-25-0		7.6					77	new
m-diisopropylbenzene	C12H18	99-62-7	-3.0						3	[27]
							-12		3	
n-hexylbenzene	C12H18	1077-16-3						26	2	
								26	3	[8]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
diphenylmethane	C13H12	101-81-5					11		3,4	[8]
n-propyltetralin	C13H18							8	3,4	[8]
n-heptylbenzene	C13H20	1078-71-3						35	2	
								34	3	
								35	3	[8]
1,2-diphenylethane	C14H14	103-29-7	1.0						3,4	[27]
dibenzyl ether	C14H14O	103-50-4		8.1					76	new
1-butylnaphthalene	C14H16	1634-09-9						6	7	
1-n-butylnaphthalene	C14H16	1634-09-9						6	3,4	[8]
2-(1,1-dimethylethyl)-naphthalene	C14H16	2876-35-9						3	3,4	[8]
?cis-n-butyltetralin	C14H20							18	3,4	[8]
?trans-n-butyltetralin	C14H20							14	3	
sec-butyltetralin	C14H20							7	3,4	[8]
tert-butyltetralin	C14H20							17	3,4	[8]
2-phenyloctane	C14H22	777-22-0						33	3,4	[8]
n-octylbenzene	C14H22	2189-60-8						43	2	
								32	3,4	[8]
1,3,5-triisopropylbenzene	C15H24	717-74-8		2.8					41	[12]
n-nonylbenzene	C15H24	1081-77-2						50	7	
								50	3,4	[8]
n-octylxylene	C16H26							20	3,4	[8]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2-methyl-2-(beta-naphthyl)hexane	C17H22							10	3,4	[8]
2-phenyl-2-undecene	C17H26							23	3,4	[8]
2-phenylundecane	C17H28	4536-88-3						51	3,4	[8]
2-octylnaphthalene	C18H24	2876-44-0						18	7	
								18	3,4	[8]
4-methyl-4-(2-naphthyl)heptane	C18H24							9	3,4	[8]
n-octyltetralin	C18H28							18	3,4	[8]
4-phenyldodecane	C18H30	2719-64-4						42	3,4	[8]
n-dodecylbenzene	C18H30	123-01-3						68	3,4	[8]
7-phenyltridecane	C19H32	2400-01-3						41	3,4	[8]
3,6-dimethyl-3-(beta-naphthyl)octane	C20H28							18	3,4	[8]
5-methyl-5-(beta-naphthyl)nonane	C20H28							12	3,4	[8]
2-phenyltetradecane	C20H34	4534-59-2						49	3,4	[8]
n-tetradecylbenzene	C20H34	1459-10-5						72	3	[8]
								72	7	
2-methyl-2-(beta-naphthyl)decane	C21H30							18	3,4	[8]
3-ethyl-3-(beta-naphthyl)nonane	C21H30							13	3,4	[8]
2-methyl-2-phenylpentadecane	C22H38	29138-94-1						39	3,4	[8]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2-methyl-4-isobutyl-4-phenylundecane	C22H38							18	3,4	[8]
2-methyl-2-phenylheptadecane	C24H42							39	3,4	[8]
5-butyl-5-phenyltetradecane	C24H42							58	3,4	[8]
1,2,4-trimethyl-5-hexadecylbenzene	C25H44							42	3,4	[8]
di-n-octyltetralin	C26H44							26	3,4	[8]
5-phenyleicosane	C26H46	2400-04-6						39	3,4	[8]

A.4 Alcohols

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
methanol	CH4O	67-56-1						5	15	
								2	37	
								3	13,14	
ethanol	C2H6O	64-17-5				12			17	
							2		57	[6]
								2	16	
								11	36	
								8	13,47	
n-propanol	C3H8O	71-23-8						12	36	
2-methoxyethanol	C3H8O2	109-86-4		15.5					76	new
2-butanol	C4H10O	78-92-2		8.5					57	
ethylene glycol vinyl ether	C4H8O2	764-48-7		14.0					76	new
isobutanol	C4H10O	78-83-1		8.5					57	
n-butanol	C4H10O	71-36-3		12.0					57	
					3.7				65	
								17	36	
t-butanol	C4H10O	75-65-0					6		57	[6]
1-methoxy-2 propanol	C4H10O2	107-98-2		16.3					76	new
cyclopentanol	C5H10O	96-41-3		9.8					76	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1-pentanol	C5H12O	71-41-0	18.2						18	
								20	36	
2-methyl-2-butanol	C5H12O	75-85-4		12.1					76	new
3-methyl-1-butanol	C5H12O	123-51-3		13.1					76	new
isopentanol	C5H12O	6423-06-9		18.4					41	
2-isopropoxyethanol	C5H12O2	109-59-1		27.8					76	new
cyclohexanol	C6H12O	108-93-0		16.3					76	new
4-hydroxy-4-methyl-2-pentanone	C6H12O2	123-42-2		11.5					76	new
1-hexanol	C6H14O	111-27-3	23.3						18	
3-methoxy-3-methyl-1-butanol	C6H14O2	56539-66-3		10.0					76	new
1-heptanol	C7H16O	111-70-6	29.5						18	
				29.0					41	
2-heptanol	C7H16O	543-49-7		25.0					41	new
4-heptanol	C7H16O	589-55-9		21.0					41	new
guaiacol	C7H8O2	90-05-1		19.3					69	new
2-phenyl ethanol	C8H10O	60-12-8		8.0					69	new
1,2 dimethoxybenzene	C8H10O2	91-16-7		17.0					69	new
4-methyl guaiacol	C8H10O2	93-51-6		19.8					69	new
2,6-dimethoxyphenol	C8H10O3	91-10-1		26.0					69	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1-octanol	C8H18O	111-87-5	39.1						18	
				33.7					41	[2]
				33.9					76	new
2-ethyl-1-hexanol	C8H18O	104-76-7		23.5					41	
3-octanol	C8H18O	589-98-0		25.1					41	
4-propyl phenol	C9H12O	645-56-7		8.6					70	new
4-propylphenol	C9H12O	645-56-7		8.6					69	new
4-ethyl guaiacol	C9H12O2	2785-89-9		19.6					69	new
4-methyl-2,6-dimethoxyphenol	C9H12O3	6638-05-7		25.0					69	new
1-nonanol	C9H20O	143-08-8	46.2						18	
2-nonanol	C9H20O	628-99-9		39.6					41	
4-nonanol	C9H20O	5932-79-6		28.0					41	new
4-propylguaiacol	C10H14O2	2785-87-7		18.0					69	new
geraniol	C10H18O	106-24-1		22.0					41	new
				16.5					76	new
linalool	C10H18O	78-70-6		20.0					41	new
				12.9					76	new
β-citronellol	C10H20O	106-22-9		25.6					41	
1-decanol	C10H22O	112-30-1	50.3						18	
3,7-dimethyl-1-octanol	C10H22O	106-21-8		29.3					41	
1-undecanol	C11H24O	112-42-5	53.2						18	
1-dodecanol	C12H26O	112-53-8	63.6						18	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
1-tetradecanol	C14H30O	112-72-1	80.8						18	
farnesol	C15H26O	4602-84-0		24.0					41	new
nerolidol	C15H26O	7212-44-4		19.2					76	new
palmitoleyl alcohol	C16H32O	10378-01-5				46			19	
1-hexadecanol	C16H34O	36653-82-4				68			19	
linolenyl alcohol	C18H32O	506-44-5				41			19	
linoleyl alcohol	C18H34O	506-43-4				44			19	
oleyl alcohol	C18H36O	143-28-2				51			19	
1-octadecanol	C18H38O	112-92-5				81			19	[5]

A.5 Aldehydes/Ketones

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
butanal	C4H8O	123-72-8		41.1					76	new
isobutyraldehyde	C4H8O	78-84-2		21.1					76	new
cyclopentanone	C5H8O	120-92-3		9.0					41	new
3-pentanone	C5H10O	96-22-0		9.7					41	new
				19.5					76	new
valeraldehyde	C5H10O	110-62-3		67.9					41	new
				62.2					76	new
cyclohexanone	C6H10O	108-94-1						10	47	
				10.4					76	new
4-methyl-2-pentanone	C6H12O	108-10-1		12.6					76	new
hexanal	C6H12O	66-25-1		75.2					76	new
3-cyclohexene-1-carboxaldehyde	C7H10O	100-50-5		28.1					76	new
cycloheptanone	C7H12O	502-42-1		22.5					76	new
2,4-dimethyl-3-pentanone	C7H14O	565-80-0		15.8					76	new
				13.0					41	new
2-heptanone	C7H14O	110-43-0		30.0					41	
2-octanone	C8H16O	111-13-7		36.6					76	new
3-octanone	C8H16O	106-68-3		36.0					41	[3] old value was 35.2
octanal	C8H16O	124-13-0		109					41	new
				102.5					76	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
3,3,5-trimethyl-cyclohexanone	C9H16O	873-94-9		11.9					76	new
whiskey lactone	C9H16O2	39212-23-2		27.2					76	new
2-nonanone	C9H18O	821-55-6		46.1					76	new
4-nonanone	C9H18O	4485-09-0		43.0					41	new
menthone	C10H18O	89-80-5		20.6					76	new
δ-undecalactone	C10H18O2	705-86-2		48.6					76	new
ε-decalactone	C10H18O2	5579-78-2		40.5					76	new
γ-undecanolactone	C11H20O2	104-67-6		52.6					76	new
6-undecanone	C11H22O	927-49-1		49.0					41	new

A.6 Ethers

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
dimethyl ether	C2H6O	115-10-6						55	20	
								78	21	
2-methoxyethanol	C3H8O2	109-86-4						13	15	
dimethoxymethane	C3H8O2	109-87-5					49		24	[24]
								29	23	
								50	25	
								55	37	
diethyl ether	C4H10O	60-29-7				160			23	
								140	37	
1,2-dimethoxyethane	C4H10O2	110-71-4						90-98	26	
				81.0					76	new
1-methoxy-2 propanol	C4H10O2	107-98-2					19		24	[24]
poly(oxymethylene) dimethyl ethers	C4H10O3							63	53	
2,3-dihydrofuran	C4H6O	1191-99-7		20.0					72	new
2,5-dihydrofuran	C4H6O	1708-29-8		15.6					72	new
tetrahydrofuran	C4H8O	109-99-9		21.9					72	new
				21.9					76	new
3,4-dihydro-2H-pyran	C5H8O	110-87-2		23.9					76	new
2-methyl tetrahydrofuran	C5H10O	96-47-9		22.0					72	new
				21.3					76	new
tetrahydropyran	C5H10O	142-68-7		38.2					76	new
2-tetrahydrofurfuryl alcohol	C5H10O2	97-99-4		17.9					72	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
2,2-dimethoxypropane	C5H12O2	77-76-9		31.3					76	new
diethylene glycol monomethyl ether	C5H12O3	111-77-3		38.3					76	new
poly(oxymethylene) dimethyl ethers	C5H12O3							70	53	
ethyl acetoacetate	C6H10O3	141-97-9		13.7					76	new
cyclopentyl methyl ether	C6H12O	5614-37-9		47.3					76	new
2-ethyl tetrahydrofuran	C6H12O	1003-30-1		28.1					72	new
2-ethoxyethyl acetate	C6H12O3	111-15-9					40		24	[24]
1,1-diethoxy ethane	C6H14O2	105-57-7		40.0					71	new
								40	56	
				54.1					76	new
2-butoxyethanol	C6H14O2	111-76-2					41		24	[24]
								35	27	
diethoxymethane	C6H14O2	462-95-3		57.3					76	new
2-methoxyethyl ether	C6H14O3	111-96-6				170			23	
							109		28	
								>100	15	
								112-130	26	[16],[23]
								126	27	
diisopropyl ether	C6H14O3	108-20-3		23.6					76	new
poly(oxymethylene) dimethyl ethers	C6H14O3							90	53	
2,4,7,9-tetra-oxa-decane	C6H14O4						58		24	[15],[24]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
anisole	C7H8O	100-66-3		6.4					69	new
tetrahydrofurfuryl acetate	C7H12O3	637-64-9		18.2					76	new
ethyl tetrahydrofurfuryl ether	C7H14O2	62435-71-6		78.9					41	new
hexylmethyl ether	C7H16O	4747-07-3		99.8					41	
1-butoxy-2-propanol	C7H16O2	5131-66-8		36.1					41	[2]
dipropylene glycol monomethyl ether	C7H16O3	252-104-2		43.9					41	[2]
							44		24	[24]
					52.0				67	[38]
triethylene glycol monomethyl ether	C7H16O4	112-35-6		80.7					41	
4-methoxy-benzaldehyde	C8H8O2	123-11-5		25.8					76	new
4-methyl anisole	C8H10O	104-93-8		7.4					69	new
1,2-dimethoxybenzene	C8H10O2	91-16-7		9.8					76	new
2-butyl tetrahydrofuran	C8H16O	1004-29-1		45.5					72	new
dibutyl ether	C8H18O	142-96-1						91-100	26	[16],[23]
				115.4					76	new
diisobutylether	C8H18O	628-55-7		59.7					41	[2]
diethoxybutane	C8H18O2						97		29	
dimethoxyhexane	C8H18O2						88		29	
2-ethoxyethyl ether	C8H18O3	112-36-7					151		24	[24]
								113-133	26	[16],[23]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
triethyleneglycol dimethyl ether	C8H18O4	112-49-2						120	47	
dibutoxymethane	C9H20O2	2568-90-3						74	25	
4-propylanisole	C10H14O	104-45-0		7.5					69	new
eucalyptol	C10H18O	470-82-6		18.8					76	new
diisoamylether	C10H22O	544-01-4		96.3					41	
				96.0					41	new
dipentyl ether	C10H22O	693-65-2						111-130	26	[16],[23]
				111.0					41	new
tripropylene glycol monomethyl ether	C10H22O4	25498-49-1		81.3					41	
							63		24	[15],[24]
								65	47	
rose oxide	C10H8O	16409-43-1		30.0					41	
1,4-cyclohexane-dimethanol divinyl ether	C12H20O2	17351-75-6		61.1					76	new
dodecyl vinyl ether	C14H30O			101.7					76	new

A.7 Esters

A.7.1 Esters: Saturated

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
methyl acetate	C3H6O2	79-20-9		19.5					76	new
methyl butanoate	C5H10O2	623-42-7	6.4						66	
							6		64	[6]
methyl levulinate	C6H10O3	624-45-3		7.8					41	new
methyl pentanoate	C6H12O2	624-24-8		13.3					58	
propylene glycol monomethyl ether acetate	C6H12O3	108-65-6		24.0					76	new
ethyl levulinate	C7H12O3	539-88-8		6.0					41	new
ethyl pentanoate	C7H14O2	539-82-2		18.6					58	
methyl caproate	C7H14O2	106-70-7	18.0						18	
				23.9					41	
				25.3					76	new
pentyl acetate	C7H14O2	628-63-7		23.6					41	new
butyl butanoate	C8H16O2	109-21-7		17.8					41	
ethyl hexanoate	C8H16O2	123-66-0		27.5					76	new
				28.0					41	new
hexyl acetate	C8H16O2	142-92-7		32.2					76	new
n-hexyl acetate	C8H16O2	142-92-7		33.8					41	
methyl heptanoate	C8H16O2	106-73-0		34.2					41	[2]
propyl pentanoate	C8H16O2	141-06-0		20.7					58	
butyl levulinate	C9H16O3	2052-15-5		14.4					41	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
butyl pentanoate	C9H18O2	591-68-4		23.5					58	
methyl octanoate	C9H18O2	111-11-5	33.6						31	[37]
								34	22	
				39.8					68	new
butyl hexanoate	C10H20O2	626-82-4		31.0					41	new
ethyl octanoate	C10H20O2	106-32-1		42.2					68	new
hexyl butyrate	C10H20O2	2639-63-6		29.0					41	new
pentyl pentanoate	C10H20O2	2173-56-0		28.8					41	
				27.6					58	
				30.0					70	new
methyl decanoate	C11H22O2	110-42-9	47.9						18	
			47.2						31	
				52.7					41	[7]
				50.7					41	
				51.6					42	
				54.1					64	
					52.1				65	
				51.6					68	new
butyl octanoate	C12H24O2	589-75-3	39.6						31	
decyl acetate	C12H24O2	112-17-4					62		32	[21],[26]
ethyl decanoate	C12H24O2	110-38-3	51.2						31	
							60		32	[21],[26]
				54.6					68	new
hexyl hexanoate	C12H24O2	6378-65-0		40.0					41	new

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
isopropyl decanoate	C13H26O2	2311-59-3	46.6						31	
methyl laurate	C13H26O2	111-82-0	61.2						12	[37]
			60.8						18	[37]
			61.4						31	
				66.7					42	
				66.3					41	
						54			24	
							70		32	[21],[26]
				66.7					68	new
octyl valerate	C13H26O2	5451-85-4					49		32	[21],[26]
propyl decanoate	C13H26O2	30673-60-0	52.9						31	
							64		32	[21],[26]
butyl decanoate	C14H28O2	30673-36-0	54.6						31	
							63		32	[21],[26]
dodecyl acetate	C14H28O2	112-66-3					77		32	[21], [26]
ethyl laurate	C14H28O2	106-33-2					73		32	[21],[26]
decyl valerate	C15H30O2	5454-12-6					61		32	[21],[26]
methyl myristate	C15H30O2	124-10-7	73.5						18	
			66.2						31	
							72		32	[21],[26]
				75.8					76	new
propyl laurate	C15H30O2	3681-78-5					71		32	[21],[26]
butyl laurate	C16H32O2	106-18-3					73		32	[21],[26]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
ethyl myristate	C16H32O2	124-06-1	66.9						31	
							72		32	[21],[26]
hexyl caprate	C16H32O2	10448-26-7					64		32	[21],[26]
tetradecyl acetate	C16H32O2	638-59-5					81		32	[21],[26]
dodecyl valerate	C17H34O2						67		32	[21],[26]
methyl palmitate	C17H34O2	112-39-0	74.5						31	[5]
			74.3						12	[37]
			74.3						18	[5]
				85.9					42	[5]
						91			19	[5]
						86			33	[5]
							80		32	[21], [5], [26]
propyl myristate	C17H34O2	14303-70-9					71		32	[21],[26]
butyl myristate	C18H36O2	110-36-1	69.4						31	
							73		32	[21],[26]
ethyl palmitate	C18H36O2	628-97-7				93			33	
							80		32	[21],[26]
hexadecyl acetate	C18H36O2	629-70-9					86		32	[21],[26]
hexyl laurate	C18H36O2	34316-64-8					74		32	[21],[26]
isopropyl palmitate	C19H38O2	142-91-6				83			33	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
methyl stearate	C19H38O2	112-61-8	86.9						12	[37]
			75.6						18	
				95.6					41	[20]
						100			19	
						101			33	[23]
							87		31	[29],[31]
							81		32	[21], [23],[26]
propyl palmitate	C19H38O2	2239-78-2					83		32	[21],[26]
						85			33	
tetradecyl valerate	C19H38O2						68		32	[21],[26]
2-butyl palmitate	C20H40O2					85			33	
butyl palmitate	C20H40O2	111-06-8				92			33	
							87		32	[21],[26]
decyl caprate	C20H40O2	1654-86-0					81		32	[21],[26]
ethyl stearate	C20H40O2	111-61-5	76.8						12	[37]
							86		32	[21],[26]
						98			33	
						77			34	
hexyl myristate	C20H40O2	42231-99-2					72		32	[21],[26]
isobutyl palmitate	C20H40O2	110-34-9				84			33	
octadecyl acetate	C20H40O2	822-23-1					90		32	[21],[26]
octyl laurate	C20H40O2	5303-24-2					84		32	[21],[26]
hexadecyl valerate	C21H42O2	125164-54-7					70		32	[21],[26]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
isopropyl stearate	C21H42O2	112-10-7				97			33	
methyl arachidate	C21H42O2	1120-28-1				100			19	
propyl stearate	C21H42O2	3634-92-2				91			33	
						70			34	
2-butyl stearate	C22H44O2	123-95-5				98			33	
butyl stearate	C22H44O2	123-95-5				93			33	
						80			34	
decyl laurate	C22H44O2	36528-28-6					84		32	[21],[26]
hexyl palmitate	C22H44O2	42232-25-7					87		32	[21],[26]
isobutyl stearate	C22H44O2	646-13-9				99			33	
octyl myristate	C22H44O2	16260-26-7					71		32	[21],[26]
2-ethylhexyl palmitate	C24H48O2	16958-85-3					107		32	[21],[26]
						98			33	
decyl myristate	C24H48O2	41297-71-3					72		32	[21],[26]
dodecyl laurate	C24H48O2	13945-76-1					85		32	[21],[26]
2-ethylhexyl stearate	C26H52O2	22047-49-0				116			33	
decyl palmitate	C26H52O2	42232-27-9					91		32	[21],[26]
dodecyl myristate	C26H52O2	2040-64-4					74		32	[21],[26]
hexadecyl laurate	C28H56O2	8038-55-9					88		32	[21],[26]

A 7.2 Esters: Unsaturated

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
methyl sorbate	C7H10O2	689-89-4		6.0					41	
methyl-9-decenoate	C11H20O2			38.3					41	[7]
vinyl laurate	C14H26O2	2146-71-6		77.0					76	new
methyl palmitoleate	C17H32O2	1120-25-8				51			33	
				56.6					68	new
methyl linolenate	C19H32O2	301-00-8	45.9						12	[36]
						23			34	
				37.0					41	[2]
methyl α-linolenate	C19H32O2			22.7					46	
methyl γ-linolenate	C19H32O2			29.2					45	
methyl linoleate	C19H34O2	112-63-0	41.7						12	[35]
				43.9					41	[2]
				38.2					42	
						38			33	
						42			34	
								43	22	
methyl linolelaidate	C19H34O2	2566-97-4		43.0					46	
methyl elaidate	C19H36O2	1937-62-8		57.2					46	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
methyl oleate	C19H36O2	112-62-9	56.0						12	[35]
				59.8					41	[2], [20]
				56.6					42	
				59.3					42	
						80			19	
						59			33	
						55			34	
							71		32	[21], [26]
								53	22	
				56.6					68	new
methyl petroselinate	C19H36O2	2777-58-4		58.6					46	
methyl ricinoleate	C19H36O3	141-24-2		37.4					68	new
				37.4					42	
methyl asclepate	C19H38O2			53.9					46	
ethyl linolenate	C20H34O2	1191-41-9				27			34	
ethyl linoleate	C20H36O2	544-35-4	44.4						12	[35]
						40			33	
						37			34	
ethyl oleate	C20H38O2	111-62-6				68			33	
						54			34	
							72		32	[21], [26]
methyl-5(Z)8(z)11(Z)14(Z)-eicosatetraenoate	C21H34O2			29.6					44	
propyl linolenate	C21H36O2					27			34	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
propyl linoleate	C21H38O2	38433-95-3				44			33	
						41			34	
isopropyl oleate	C21H40O2	112-11-8				87			33	
methyl gondoate	C21H40O2	2390-09-2		73.2					43	
propyl oleate	C21H40O2	111-59-1					72		32	[21], [26]
						59			33	
						56			34	
butyl linolenate	C22H38O2					29			34	
						42			34	
butyl linoleate	C22H40O2					54			33	
2-butyl oleate	C22H42O2					72			33	
butyl oleate	C22H42O2	142-77-8				60			34	
						62			33,35	
							102		32	[21], [26]
isobutyl oleate	C22H42O2	10024-47-2				60			33	
methyl 4(Z),7(Z),10(Z),13(Z), 16(Z),19(Z)-docosahexaenoate	C23H34O2	28061-46-3		24.4					44	
methyl erucate	C23H44O2	1120-34-9		74.2						
hexyl oleate	C24H46O2	20290-84-0					102			
2-ethylhexyl oleate	C26H50O2	26399-02-0				88			33	
octyl oleate	C26H50O2	32953-65-4					131		32	[21],[26]
decyl oleate	C28H54O2	3687-46-5					134	43		[21], [23], [26]

A.7.3 Esters: Diesters/Triglycerides

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
dimethyl malonate	C5H8O4	108-59-8					15		32	[21],[26], [37]
diethyl oxalate	C6H10O4	95-92-1					21		32	[21],[26], [37]
diethyl malonate	C7H12O4	105-53-3					15		32	[21],[26], [37]
diethyl butanedioate	C8H14O4	123-25-1	21.0						52	[18]
diethyl succinate	C8H14O4	627-93-0					14		32	[21],[26], [37]
dimethyl adipate	C8H14O4	105-99-7					5		32	[21],[26], [37]
glycerol triacetate	C9H14O6	102-76-1		<5					41	[17]
dimethyl phthalate	C10H10O4	131-11-3					19		32	[21],[26], [37]
diethyl adipate	C10H18O4	141-28-6					15		24	[24]
dibutyl malonate	C11H20O4	1190-39-2	21.0						52	[18]
dimethyl azelate	C11H20O4	1732-10-1					24		32	[21],[26], [37]
dibutyl butanedioate	C12H14O4	141-03-7	21.0						52	[18]
dibutyl butanedioate	C12H14O4	141-03-7	21.0						52	[18]
dibutyl fumarate	C12H20O4	105-75-9	23.0						52	[18]

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
dibutyl maleate	C12H20O4	105-76-0					29		24	[24]
								28	47	
diethyl azelate	C13H24O4	624-17-9					47		32	[21],[26], [37]
diethyl sebacate	C14H26O4	110-40-7					47		32	[21],[26], [37]
dibutyl adipate	C14H26O4	105-99-7					81		32	[21],[26], [37]
tributyrin	C15H26O6	60-01-5					-5		24	[24]
dibutyl phthalate	C16H22O4	87-74-2					38		32	[21],[26], [37]
dibutyl azelate	C17H32O4	2917-13-9					83		32	[21],[26], [37]
dihexyl phthalate	C20H30O4	84-75-3					48		32	[21],[26], [37]
dibutyl succinate	C12H22O4	141-03-7			13.0				67	
dihexyl azelate	C21H40O4	109-31-9					99		32	[21],[26], [37]
dioctyl adipate	C22H42O4	123-79-5					89		32	[21],[26], [37]
dioctyl sebacate	C26H50O4	122-62-3					70		32	[21],[26], [37]
trilaurin	C39H74O6	538-24-9				100			19	
trimyristin	C45H86O6	555-45-3				100			19	

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
tripalmitin	C51H98O6	555-44-2				89			19	
triolein	C57H104O6	122-32-7				45			19	
tristearin	C57H110O6	555-43-1				85			19	
trilinolenin	C57H92O6	14465-68-0				23			19	
trilinolein	C57H98O6	537-40-6				32			19	

A.8 Acids

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
decanoic acid	C10H20O2	334-48-5					48		31	[29], [31]
linolenic acid	C18H30O2	463-40-1				20			34	
linoleic acid	C18H32O2	60-33-3				31			34	
oleic acid	C18H34O2	112-80-1				46			34	
stearic acid	C18H36O2	57-11-4				62			34	[5]

A.9 Furans

Compound	Formula	CAS	ASTM Method D613 (CFR)	ASTM Method D6890 (IQT)	ASTM Method D7170 (FIT)	Other Ignition Delay Method	Blend	Unknown Method	Ref.	Notes
furan	C4H4O	110-00-9		7.0					72	new
furfural	C5H4O2	98-01-1		13.9					76	new
2-methyl furan	C5H6O	534-22-5		8.9					72	new
				9.1					76	new
2-furfuryl alcohol	C5H6O2	98-00-0		10.8					72	new
				9.7					76	new
2,5 dimethyl furan	C6H8O	625-86-5		10.9					72	new
2-ethyl furan	C6H8O	3208-16-0		10.2					72	new
2-butyl furan	C8H12O	4466-24-4		13.1					72	new
furfuryl ethyl ether	C7H10O2	6270-56-0		18.4					41	new

Notes

[1] 20% blend.

[2] All new data updated to use D6890-06 DCN correlation: DCN = 4.460 + 186.6/ignition delay (except when ignition delay is outside range of 3.3 to 6.4 milliseconds, then use original equation) including data collected before spec came into effect.

[3] Data already in Compendium, also updated with new correlation between ignition delay for IQT in ASTM D6890-06 and later versions.

[4] Primary reference fuel, value set by ASTM D6890 for IQT.

[5] Compound solid at room temperature, must be heated to test.

[6] Blend tested on IQT.

[7] Compound was treated with silica gel to remove contaminants.

[8] Calculated from cetene value × 0.875.

[9] Primary reference fuel value set by ASTM D613 for CFR.

[10] cis-Isomer surmised from boiling point and density data.

[11] Original reference says this is an "extrapolated value."

[12] Estimated DCN is Y-intercept from regression of compound blends with n-heptane.

[13] Sample contained oxidation inhibitor.

[14] Original source states: “These compounds are apparently two isomers on n-butyltetralin,” but does not specify which is which.

[15] Because of small difference in blend CN and base fuel CN, blend calculation is not very meaningful.

[16] Delay values are from correlations with reference fuels and with diesel fuels, respectively.

[17] Actual value may be much less than 5.

[18] ISO 5165, European equivalent to ASTM D613.

[19] Value is from double blend procedure with potential for large errors.

[20] Fuel reservoir and line heated to 55°C.

[21] Used BASF engine and DIN 51773.

[22] Reference says cetane number collected by "engine method."

[23] Cetane number changed from 2004 Compendium.

[24] Based on approx. 20% blend.

[25] Based on a 30% blend.

[26] Based on a 5%–7% blend.

[27] Measured using ASTM D613-43T (a temporary version of standard).

[28] Based on 80% blend.

[29] Based on 70% blend.

[30] Measured using ASTM D613-59T (a temporary version of the standard).

[31] Blend tested using ASTM D613.

[32] From 14 ternary mixtures of n-decane, iso-octane, and toluene.

[33] From 43 mixtures of n-dodecane/iso-octane/1,3,5-trimethylbenzene/n-propylbenzene.

[34] Optimized from [32] and another set of 15 blends.

[35] Test method changed from 2004 Compendium.

[36] Name of compound changed from 2004 Compendium.

[37] Measurement not included in 2004 Compendium, although reference had been included.

[38] Dipropylene glycol methyl ether, mixed isomers, aka DOWANOL DPM glycol ether.

Appendix B. Sources for Cetane Number Data

Number	Reference
1	Olson, D.R.; Meckel, N.T.; Quillian, R.D. (1960). "Combustion Characteristics of Compression Ignition Engine Fuel Components." SAE Technical Paper 600112. http://dx.doi.org/10.4271/600112
2	Hardenberg, H.O. (1984). "Zundwilligkeit und Cetanzahl reiner Kohlenwasserstoffe." *Mineraloeltechnik* (29); p. 13.
3	Puckett, A.D.; Caudle, B.H. (1948). *Ignition Qualities of Hydrocarbons in the Diesel Fuel Boiling Range*. Washington, DC: U.S. Department of the Interior, Bureau of Mines Information Circular 7474.
4	Rose, J.W.; Cooper, J.R., eds. (1977). "Detonation of Liquid Fuels." In *Technical Data on Fuel,* British National Committee, World Energy Conference, p. 285.
5	Hurn, R.W.; Smith, H.M. (1951). "Hydrocarbons in the Diesel Boiling Range." *Industrial and Engineering Chemistry* (43:12); pp. 2788–2793. http://dx.doi.org/10.1021/ie50504a044
6	Gulder, O.L.; Glavincevski, B.; Kallio, N.N. (1989). "A Rapid Cetane Number Prediction Method for Petroleum Liquids and Pure Hydrocarbons Using Proton NMR." SAE Technical Paper 892073. http://dx.doi.org/10.4271/892073
7	Chevron. (2007). *Diesel Fuels Technical Review FTR-2.* https://www.google.com/url?q=http://www.chevronwithtechron.ca/products/documents/Diesel_Fuel_Tech_Review.pdf&sa=U&ei=eFiGU6GSIcubyATEm4DoDQ&ved=0CCIQFjABOAo&usg=AFQjCNEbGC9eSkLXlUSKcYGid5NaGIPK-A
8	American Society for Testing and Materials. (1958). *Knocking Characteristics of Pure Hydrocarbons.* ASTM Special Technical Publication 225, developed under American Petroleum Institute Research Project 45.
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10	Petrov, A.D. (1946). "Cetene Number Data." *Bull. Acad. Sci. USSR* (4) p. 543.
11	Guibet, J.-C. (1999). *Fuels and Engines*. (1); p. 339.
12	McCormick, R.L.; Grabowski, M.S.; Alleman, T.L.; Herring, A.M.; Tyson, K.S. (2001). "Impact of Biodiesel Source Material and Chemical Structure on Emissions of Criteria Pollutants from a Heavy-Duty Engine." *Environ. Sci. Tech.* (35:9) p. 1742–1747. http://dx.doi.org/10.1021/es001636t
13	Kroeger, C.A. (1986). "A Neat Methanol Direct Injection Combustion System for Heavy-Duty Applications." SAE Technical Paper 861169. http://dx.doi.org/10.4271/861169
14	McCormick, R.L. (2002). "Technical Barriers to the Use of Ethanol in Diesel Fuel." 7th Annual National Ethanol Conference, 27 Feb–1 Mar 2002.
15	Tijm, P.J.A. (1998). "Overview of Cetaner for Diesel Fuel and an AET Study of Cetaner Blended with Low Cetane Diesel Fuel." Windsor Workshop, 8–10 June 1998.
16	Hardenberg, H.O.; Schaefer, A.J. (1981). "The Use of Ethanol as a Fuel for Compression Ignition Engines." SAE Technical Paper 811211. http://dx.doi.org/10.4271/811211

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