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Subcontractor Report

Compendium of Experimental Cetane Number Data

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Abstract

In this report, we present a compilation of reported cetane numbers for pure chemical compounds. The compiled database contains cetane values for 299 pure compounds, including 156 hydrocarbons and 143 oxygenates. Cetane number is a relative ranking of fuels based on the amount of time between fuel injection and ignition. The cetane number is typically measured either in a combustion bomb or in a single-cylinder research engine. This report includes cetane values from several different measurement techniques – each of which has associated uncertainties. Additionally, many of the reported values are determined by measuring blending cetane numbers, which introduces significant error. In many cases, the measurement technique is not reported nor is there any discussion about the purity of the compounds. Nonetheless, the data in this report represent the best pure compound cetane number values available from the literature as of August 2004.

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1 Introduction

The U.S. Department of Energy (DOE) is committed to increasing our nation's energy security by decreasing our dependence on imported petroleum. The Fuels Technologies Subprogram within DOE's Office of FreedomCAR and Vehicle Technology (OFCVT) supports research that allows the United States to develop advanced fuels that enable efficient engines with low emissions. Understanding how the molecular composition of fuels impacts ignition properties will lead to improved fuel formulations that enable higher efficiency engine operation.

Fuels for compression ignition engines must ignite readily through autoignition alone. If ignition does not occur promptly when the fuel is injected into the cylinder, unburned fuel will accumulate as the injection process proceeds. In addition, when ignition does occur, the rate of burning will be too rapid, resulting in engine knock that decreases efficiency while increasing engine noise and wear. Thus, the ability to rate the ignition quality of compression ignition fuels is important to diesel fuel formulation. Without adequate fuel ignition quality the engine will start with difficulty and run poorly.

This report presents all available experimental cetane number data for pure compounds as of August 2004. The report also 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 for inclusion in future editions.*

1.1 Compression Ignition Background

When operating a compression ignition engine, a 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 to approximately 600° C. At this time, liquid fuel is injected into the cylinder through a nozzle. The fuel forms a spray of droplets, which vaporize, mix with hot air, and ignite.

1.1.1 Physical Processes of Compression Ignition

Hydrocarbon combustion occurs only in the gas phase. Thus, for a liquid fuel, the first steps toward ignition involve transitioning from a liquid to a gas phase. 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]

- density and temperature of 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.

1.1.2 Chemical Processes of Compression Ignition

Combustion is a sequence of chemical reactions in which the gas-phase fuel reacts with oxygen. These reactions proceed stepwise, through a mechanism involving free radicals.* For ignition to occur, the fuel must be heated to a temperature sufficient for some of the weaker bonds 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).

1.1.3 Complete Ignition Process

The role of these fuel properties in the various physical and chemical steps in the compression ignition process is summarized in Figure 1.

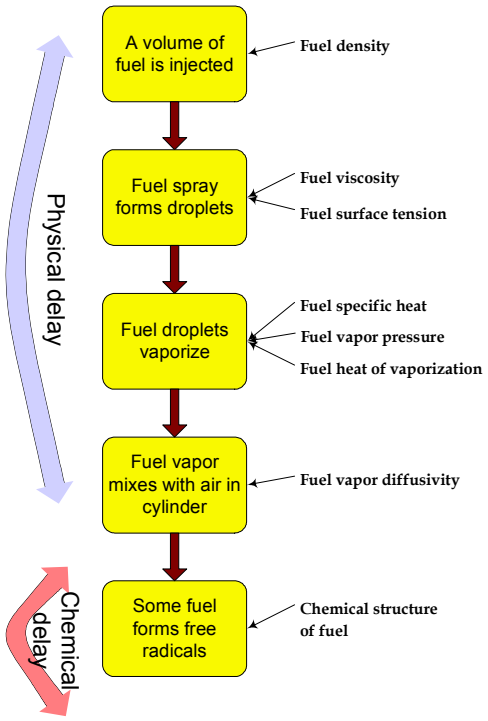

Figure 1. Overall Compression Ignition Process

Early work by Yu, Uyehara, and Myers[2] was able to show the separate effects of physical and chemical ignition delay. For all but very heavy fuels, the physical delay is short compared to the chemical delay.

* A free radical is a chemical entity containing an unpaired electron.

2 Engine Methods for Measuring Diesel Fuel Ignition Quality

The earliest evaluations of diesel fuels were most likely audible; some fuels caused the engine to operate more smoothly than others. (And the prevalence of steam engines must have offered a ready comparison between diesel engine noise and the smooth expansion of steam in the cylinder of a steam engine). Therefore, a quantitative scale was needed to rank the fuels.

2.1 Selection of Reference Fuels for a Cetane Number Scale

2.1.1 Cetene (Ketene) Rating Scale

During the 1930s, Boerlage and Broeze[3] 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-methyl naphthalene.

The first reference fuel, 1-hexadecene, also known as cetene or ketene and formally known as 1-hexadecene, has a long, straight chain structure as shown in Figure 2, and oxidizes relatively easily. This fuel was assigned a cetene (ketene) number of 100.

The second reference fuel, α-methyl naphthalene, also known as 1-methylnaphthalene, has two aromatic rings, as shown in Figure 3, and is highly resistant to oxidation. 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.

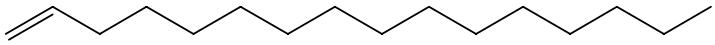

Figure 2. Structure of 1-Hexadecene (Cetene or Ketene)

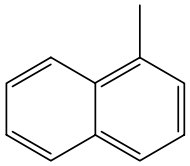

Figure 3. Structure of α-Methylnaphthalene

2.1.2 Cetane Rating Scale

Later, a similar test was used in the United States, but, because of the difficulty of preparing pure cetene,* n-hexadecane (cetane) was used as a reference fuel instead of cetene. The structure of

* It was difficult to ensure all of the hexadecene had the double bond in the one position. Moreover, hexadecene is prone to oxidation during storage.

cetane is shown in Figure 4. A comparison of the two ratings showed the following approximate relationship between cetane rating and cetene (ketene) rating:

$$\text{Cetane Rating} = 0.88 * \text{Cetene Rating}$$

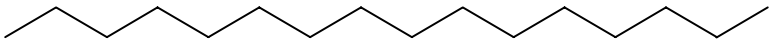

Figure 4. Structure of n-Hexadecane (Cetane)

Because of experimental difficulties in working with α-methylnaphthalene,* the reference fuel for the lower end of the cetane number scale was later changed to 2,2,4,4,6,8,8-heptamethylnonane†, shown in Figure 5, with an assigned cetane number of 15. In terms of these two reference fuels, the cetane number scale is then defined as follows:

$$CN = \%\text{ by volume hexadecane} + 0.15 * (\%\text{ by volume heptamethylnonane})$$

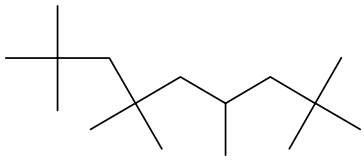

Figure 5. Structure of heptamethylnonane

2.1.3 ASTM D 613 Cetane Number Scale

The ASTM D 613 Standard Test Method of Diesel Fuel Oil now defines the cetane number scale. The method was first published in 1941, and has changed little since, with the exception of substituting heptamethylnonane, with an assigned cetane number of 15, for α-methylnaphthalene at the lower end of the scale.

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[3] proposed a method using a single-cylinder diesel CFR‡ engine with a prechamber, injecting the fuel 10 crank angle degrees (CAD) before top dead center (TDC) and adjusting a plunger in the prechamber to obtain ignition at 1 CAD after TDC, for an ignition delay of 11 CAD.§ This method formed the basis for developing the ASTM D 613 standard for cetane number.

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* α-methyl naphthalene is a suspected carcinogen and has a foul odor.

† The name of this hydrocarbon is often abbreviated to just heptamethylnonane.

‡ CFR stands for Cooperative Fuel Research, and is a standardized engine manufactured by Waukesha.

§ When this method was developed into the ASTM D 613 test, the standard ignition delay was changed to 13 degrees of CA.

In the ASTM D 613 test, the cetane number of a diesel fuel is determined by comparing its ignition delay characteristics in a 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. There is also a very similar method for determining cetane number that uses a standard BASF engine (DIN 51773). Some European cetane number data have been determined using this method.

2.3 Accuracy of Cetane Number Determinations

The current ASTM D 613 procedure lists reproducibility limits that vary from 2.8 cetane numbers at a cetane number level of 40 to 3.8 cetane numbers at a cetane number level of 48 to 4.8 cetane numbers at a cetane number level of 56. The 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 1 case in 20. In other words, for tests on a cetane number 48 fuel by multiple laboratories, 95% of the test results would be between 44.2 and 51.8. Despite the great efforts over the years to make cetane number determinations accurate, cetane numbers are not as accurate as desired.

3 Bench Methods for Measuring Diesel Fuel Ignition Quality

3.1 Early Bench Methods

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,[4] however, Falk did not measure the variation of cylinder pressure with time and so did not notice any ignition delay. Later, in 1914, Dixon *et al.*[5] recognized the existence of an ignition delay period.

Mullins[6] reports that in 1932 Helmore and Code Holland developed an ignition bomb 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 ms. Nonetheless, they observed some agreement with the behavior of test fuels in a diesel engine.

Work by Hurn and Hughes[7] 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.

3.2 The Ignition Quality Test (IQT)

More recently, studies of constant volume bomb combustion were undertaken by Ryan and coworkers at Southwest Research Institute with the goal of developing a new method for rating the ignition quality of diesel fuels.[8,9] 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. The ignition delay is measured as the time delay between the beginning of injector needle lift and the chamber pressure recovery point*. This resulted in a robust correlation between the observed ignition delay and the cetane number. The method has been refined, validated and commercialized by Advanced Engine Technology, Ltd. [10,11,12], and it has been approved by ASTM as Standard D 6890.

3.3 Other Bench Test Methods for Ignition Quality

A number of other bench test methods for measuring diesel fuel ignition quality have been developed over the years. Mostly, these bench tests have attempted to correlate cetane number with autoignition temperatures. No such tests have gained common use.

* Initially the pressure decreases due to cooling from fuel evaporation, but rises as combustion begins reaching the initial pressure at the pressure recovery point.

4 Discussion of Cetane Number Data

4.1 Origin of Data

Referenced sources and technical papers were sought in which cetane number data were presented for pure compounds. Based on this search (completed August 2004), the authors prepared a summary of all available cetane number data for pure compounds. The results are a compendium of cetane number data for 299 pure compounds including 156 hydrocarbons and 143 oxygenates. Some of the main data sources are discussed.

4.1.1 Key Data Sources for Hydrocarbons

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, which lists cetane number data for 105 pure compounds. However, these data are, in fact, the same cetane number values* for the same 105 compounds that are found in the *Technical Data on Fuels* book by Rose and Cooper, published in 1977.[13]

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.[14] The Bureau of Mines Circular contains references to the source of each cetane number value, and from these references we learn that cetane numbers for 84 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. (In the early days, 1-hexadecene or cetene rather than hexadecane or cetane was used as the reference fuel.) A 1938 correlation between the cetene number scale and the cetane number scale‡ was applied to "convert" Petrov's results to a cetane number value.

While much of Petrov's data appear to be of generally good quality§, there are some results that are persistent outliers and some other results that seem to defy general experience with diesel fuel chemistry.** While it is possible that these compounds have an unusual ignition chemistry, it is also possible that there were unrecognized difficulties in the synthesis of these compounds that resulted in either the presence of an impurity (particularly peroxides) or even erroneous synthesis of a compound with a different structure than the one desired. Considering that gas chromatography was not yet available for determining hydrocarbon purity and that instrumental analysis was not widely used to confirm the structures of organic molecules, an occasional error in synthesis or purification seems likely.

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

† One wonders about the state of scientific research in Russia during the WWII years.

‡ According to this correction, cetane number = cetene number x 0.875.

§ For some compounds cetene numbers from Petrov's data may be compared to cetane numbers from engine tests performed by the Bureau of Mines.

** Such as an alkane showing a lower cetane number than the corresponding olefin despite general experience to the contrary.

Thus, the majority of available data for the cetane numbers of pure hydrocarbons is not derived from engine test data according to the ASTM D 613, but is rather derived from WWII-era ignition delay measurements and the successive application of two correlations* involving the cetene number.

Another recent source, the 1998 "Diesel Fuels Technical Review" document[15] by Chevron, 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.†

4.1.2 Key Data Sources for Oxygenates

Serdari *et al.*[16] present cetane numbers for 48 esters. Knothe *et al*.[17] present cetane number data for 29 fatty acid esters. In an earlier paper, Knothe *et al*.[18] list cetane numbers derived from an ignition delay procedure for 21 esters, alcohols, and triglycerides. Freedman *et al*.[19] present data for 20 esters, alcohols, and triglycerides. There is substantial overlap between these sources in terms of compounds studied, and where there is overlap, the agreement is often poor.‡

Most data for fatty acid esters are from an ignition delay apparatus. Only a couple of values are reported to be from the D 613 engine test, and in those cases the experimental procedure is poorly documented considering that 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.

4.2 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. For example, Olson *et al*.[20] determined the cetane numbers of a number of blends of 10 or 20 volume percent of pure hydrocarbon components with a diesel fuel of known cetane number.

One problem with using blending cetane numbers is an amplification of uncertainty. Consider data from Olson *et al*. showing that the cetane number of a blend of 10 percent benzene with a base fuel of cetane number 38.3, is 36.8. Presuming that the cetane number of the blend is a linear combination of the cetane numbers of the components, we expect:

$$\text{Blend CN} = (0.9)(\text{Base Fuel CN}) + (0.1)(\text{Test Fuel CN})$$

or

$$\text{Test Fuel CN} = [(\text{Blend CN}) - (0.9)(\text{Base Fuel CN})] / 0.1$$

* First from ignition delay to cetene number and second from cetene number to cetane number.

† 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.

‡ As an example, the cetane number of butyl stearate is reported to be 80.1 by one of these sources and 92.5 by another of these sources.

It may be appreciated that for this blend level, a measurement error of $\pm$0.5 CN in the blend cetane number will cause a change of $\pm$5 cetane number units in the calculated blending cetane number. 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.

For example, Olson *et al*. list cetane number data for blends of a base diesel fuel with 1-methylnaphthalene and with hexadecane – the defined 0 and 100 points on the cetane number scale. The blending cetane numbers calculated for these compounds from the data of Olson *et al*. are –7 and 92, respectively.

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. There is evidence that the linear assumption is not always correct. For example, in their study of the cetane numbers of carboxylic esters, Serdari *et al*.[16] find the cetane numbers of methyl oleate blends appear to behave linearly, while those of ethyl laurate blends appear to behave non-linearly, as shown in Figure 6 and Figure 7, respectively. (Note also the widths of the error bars in these figures; these indicate the magnitude of the blending cetane number accuracy problem.)

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.

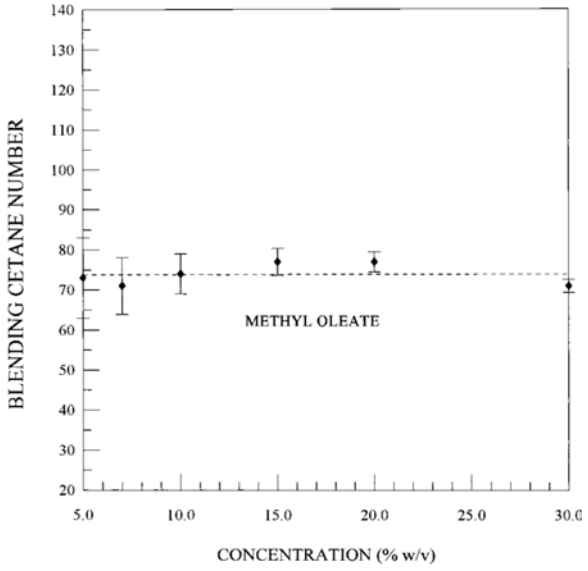

Figure 6. Blending Cetane Numbers for Various Concentrations of Methyl Oleate in Diesel Fuel [16]

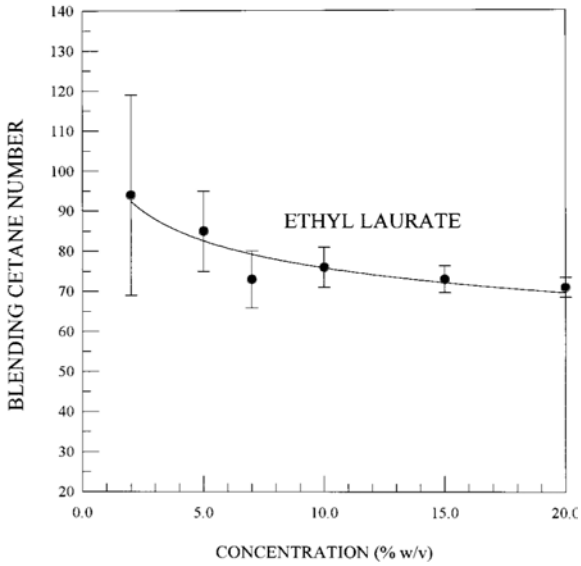

Figure 7. Blending Cetane Numbers for Various Concentrations of Ethyl Laurate in Diesel Fuel [16]

4.3 Other Issues with Cetane Number Data

4.3.1 Agreement of Duplicate Data

In instances where cetane number data are available from more than one source, there is often poor agreement; differences of 5 or 10 cetane numbers are not uncommon. This situation produces a lack of confidence in the data and raises questions about of the accuracy of the experimental methods and the purity of the compounds tested.

4.3.2 Purity of Compounds

There is little data on the purity of the compounds that were used for cetane number determinations. Because of the relatively large sample size required for the D 613 engine test, we suspect that many of the compounds had only a technical level of purity of 98% or lower. No instances were found where the identity or type of impurities was stated, nor is there data on the effect of various impurities on the measured cetane levels.

4.3.3 Presence of Peroxides

Peroxides are compounds with an R – O – O – R linkage. Most peroxides are extremely reactive and many are explosive. Peroxides have long been known to be effective additives for improving the cetane number of diesel fuels.[21]

Peroxides can be formed by the auto-oxidation of hydrocarbons in storage, and it has been found that some diesel fuels and many pure compounds can contain sufficient peroxides to affect the measured cetane number.[22] Even the n-hexadecane (cetane) diesel reference fuel can contain peroxides that affect the results of cetane number determinations.

4.3.4 Issues with Reference Compounds

The accuracy of the definition of heptamethylnonane as a primary reference fuel with a cetane number of 15 has also been called into question. In 1978 Bowden of Southwest Research Institute reported[23] that, using α-methylnaphthalene and hexadecane as reference fuels, the cetane number of heptamethylnonane was found to be only 12.2, and not 15 as is customarily assigned when it is used as a reference fuel.

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.

4.3.5 Issues with 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.

4.4 Summary of Cetane Number Data Survey

Based on this survey, we find:

- Cetane number data are available for 299 "pure" compounds.
- The purity of many of these compounds is unknown or suspect.
- In many cases duplicate data for the same compound do not agree.
- Recent results have demonstrated that the presence of peroxide impurities can make a substantial difference in the measured cetane number.
- 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.

The compendium of experimental cetane number data is included in the Appendix of this document. The compendium lists all known literature values of cetane numbers of pure compounds. The listing is organized by compound class and then by molecular formula. If the cetane number is measured using a method other than an engine test, the method used to derive the value is noted. Data from empirical cetane number correlations are not included in this compendium. Some early data are converted from cetene numbers and are noted in the Comments column.

5 Acknowledgements

The authors would like to acknowledge the U.S. Department of Energy and thank the Office of FreedomCAR and Vehicle Technologies for their support of this work. This project was funded by the Fuels Technology Subprogram in the Advanced Petroleum Based Fuels / Non-Petroleum Based Fuels activities.

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[22] "Sunlight and Air Exposure Effects on Octane Number or Cetane Number of Petroleum Product Samples," David Kohler, Randy Jennings, ASTM Research Report D02-1502, 23 Mar 2001.

[23] "Octane-Cetane Relationship," John N. Bowden, ACS Division of Fuel Chemistry Preprints, **23**, 998, (1978). p. 1005.

6 Appendix: Compendium of Experimental CN Data

In the tables that follow, several terms are used to indicate the method used as described below:

Blend = The cetane number of the pure compound is determined by measuring the cetane number of a blend of that compound with a base fuel (typically a diesel fuel) of known cetane number and then using a linear combination based on the blend composition.

Delay = The ignition delay is measured in a combustion bomb and then converted to a cetane number using a correlation for that particular device.

IQT = This is the same as a "delay" method except that a standardized piece of equipment is used and the ASTM D 6890 procedure is followed.

From ON = The octane number was measured and then a crude correlation was used to convert the octane number to a cetane number.

D 613 = The authors explicity state that the cetane number was measured using the standard CFR single-cylinder engine test method.

Blank = The method used for measuring cetane number is not explicitly stated. In many cases, the measurement technique may have been D 613, but this is not assumed.

6.1 *n-Alkanes*

Compound	Formula	CAS	CN	Method	Ref.	Comments
n-propane	C3H8	74-98-6	-20	--	37	Method unspecified.
n-butane	C4H10	106-97-8	22	from ON	11	Use ON→CN correlation in Ref 39.
n-pentane	C5H12	109-66-0	30	blend	1	For 10% blend.
n-hexane	C6H14	110-54-3	42	blend	1	For 10% blend.
			44.8	--	2	
			44.8	delay	9	
n-heptane	C6H16	142-82-5	52.5	IQT	38	
			53	blend	1	
			56	D 613	3	
			56	--	4	
n-octane	C8H18	111-65-9	63.8	--	5	
			64.4	delay	9	
			65	--	2	
n-nonane	C9H20	111-84-2	72	--	6	
			74	blend	1	
n-decane	C10H22	124-18-5	76	--	7	
			76	--	4	
			76.9	--	5	
			78	--	2	
n-undecane	C11H24	1120-21-4	79	blend	1	
			83.2	--	6	
n-dodecane	C12H26	112-40-3	80	--	3	
			80	--	4	
			87.6	--	5	

Compound	Formula	CAS	CN	Method	Ref.	Comments
n-tridecane	C13H28	629-50-5	88	--	4	
			91	--	6	
n-tetradecane	C14H30	629-59-4	93	--	4	
			95	--	2	
			95	delay	9	
			96	--	1	
			96.1	--	5	
n-pentadecane	C15H32	629-62-9	95	--	7	
			95	--	4	
			98	--	6	
n-hexadecane	C16H34	544-76-3	92	blend	1	Primary reference fuel.
			100	--	4	
n-heptadecane	C17H36	629-78-7	105	--	4	
n-octadecane	C18H38	593-45-3	102.6	--	5	
			110	--	4	
n-nonadecane	C19H40	629-92-5	110	--	4	
n-eicosane	C20H42	12-95-8	110	--	4	
			110	--	7	

6.2 *iso-Alkanes*

Compound	Formula	CAS	CN	Method	Ref.	Comments
2,2-dimethylbutane	C6H14	75-83-2	24.4	IQT	38	
2-methylpentane	C6H14	107-83-5	23	blend	1	
			33	--	4	
			34	from ON	40	Use ON→CN correlation in Ref 39.
3-methylpentane	C6H14	96-14-0	30	blend	3	
			30	--	4	
2,3-dimethylpentane	C7H16	565-59-3	21	IQT	38	
2,4-dimethylpentane	C7H16	108-08-7	29	--	1	
2,2,4-trimethylpentane	C8H18	540-84-1	12	blend	3	
			12	--	4	
			14	--	6	
			17.5	--	9	
			17.5	delay	9	
2,2,5-trimethylhexane	C9H20	3522-94-9	24	--	1	
			24	--	8	
2,2-dimethyloctane	C10H22	15869-87-1	59	--	7	
3-ethyldecane	C12H26		46	--	3	Value is cetene number x 0.875.
			48	--	10	
			48	--	7	
4,5-diethyloctane	C12H26		20	--	3	Value is cetene number x 0.875.
			20	--	7	
2,2,4,6,6-pentamethylheptane	C12H26	13475-82-6	9	--	3	Value is cetene number x 0.875.
			9	--	4	

Compound	Formula	CAS	CN	Method	Ref.	Comments
2,3,4,5,6-pentamethylheptane	C12H26	13475-82-6	9	--	11	
2,5-dimethylundecane	C13H28		58 58	-- --	3 4	Value is cetene number x 0.875.
4-propyldecane	C13H28		39 39	-- --	3 4	Value is cetene number x 0.875.
5-butylnonane	C13H28	17312-63-9	53 53	-- --	3 4	Value is cetene number x 0.875.
2,7-dimethyl-4,5-diethyloctane	C14H30		39 39	-- --	3 4	Value is cetene number x 0.875.
2,2,4,4,6,8,8-heptamethylnonane	C16H34	4-9-4390	15	--	7	Primary reference fuel
7,8-dimethyltetradecane	C16H34		40 40	-- --	3 4	Value is cetene number x 0.875.
5-butyldodecane	C16H34		45	--	4	
7-butyltridecane	C17H36		70 70	-- --	3 4	Value is cetene number x 0.875.
8-propylpentadecane	C18H38		48 48 48	-- -- --	3 4 7	Value is cetene number x 0.875.
7,8-diethyltetradecane	C18H38		67 67 67	-- -- --	3 11 4	Value is cetene number x 0.875.
9-methylheptadecane	C18H38	18869-72-2	66 66	-- --	3 4	Value is cetene number x 0.875.

Compound	Formula	CAS	CN	Method	Ref.	Comments
5,6-dibutyldecane	C18H38		30 30	-- --	3 4	Value is cetene number x 0.875.
9,10-dimethyloctadecane	C20H42		60 59	-- --	3 4	Value is cetene number x 0.875.
7-hexylpentadecane	C21H44		83 83	-- --	3 4	Value is cetene number x 0.875.
2,9-dimethyl-5,6-diisopentyldecane	C22H46		48 48	-- --	3 4	Value is cetene number x 0.875.
9,10-dipropyloctadecane	C24H50		47 47	-- --	3 4	Value is cetene number x 0.875.
9-heptylheptadecane	C24H50		88 87	-- --	3 4	Value is cetene number x 0.875.
10,13-dimethyldocosane	C24H50		56	--	11	

6.3 *Cyclo-Alkanes*

Compound	Formula	CAS	CN	Method	Ref.	Comments
cyclohexane	C6H12	110-82-7	13	--	4	
			13.15	--	3	
			13.2	--	6	
			16.9	delay	9	
			18	blend	1	
methylcyclohexane	C7H14	108-87-2	20	--	3	Value is cetene number x 0.875.
			20	--	4	
			20	--	5	
			23	IQT	38	
cyclooctane	C8H10	292-64-8	22.2	IQT	38	
ethylcyclohexane	C8H16	1678-91-7	45	from ON	8	Use ON→CN correlation in Ref 39.
n-propylcyclohexane	C9H18	1678-92-8	52	from ON	8	Use ON→CN correlation in Ref 39.
1,3,5-trimethylcyclohexane	C9H18	1839-63-0	30.5	IQT	38	
trans-decalin	C10H18	91-17-8	42.1	--	5	
			48	--	7	
			48	--	3	Value is cetene number x 0.875.
			48	--	4	
n-butylcyclohexane	C10H20	1678-93-9	46.5	IQT	38	
bicyclohexyl	C12H22	92-51-3	47.4	--	5	
			53	--	3	Value is cetene number x 0.875.
			53	--	4	

Compound	Formula	CAS	CN	Method	Ref.	Comments
3-cyclohexylhexane	C12H24		36	--	7	
			36	--	3	Value is cetene number x 0.875.
			36	--	4	
n-propyldecalin	C13H24		35	--	3	Value is cetene number x 0.875.
			35	--	4	
n-butyldecalin	C14H26		31	--	3	Value is cetene number x 0.875.
			31	--	4	
sec-butyldecalin	C14H26		34	--	3	Value is cetene number x 0.875.
			34	--	4	
tert-butyldecalin	C14H26		24	--	3	Value is cetene number x 0.875.
			24	--	4	
2-methyl-3-cyclohexylnonane	C16H32		56	--	3	Value is cetene number x 0.875.
			70	--	7	
n-octyldecalin	C18H34		31	--	3	Value is cetene number x 0.875.
			31	--	4	
4-methyl-4-decalylheptane	C18H34		21	--	3	Value is cetene number x 0.875.
			21	--	4	
1-methyl-3-dodecylcyclohexane	C19H38		70	--	3	Value is cetene number x 0.875.
			70	--	4	
3-methyl-3-decalylnonane	C20H38		18	--	3	Value is cetene number x 0.875.
			18	--	4	
2-cyclohexyltetradecane	C20H40		57	--	3	Value is cetene number x 0.875.
			57	--	4	
2-methyl-2-decalyldecane	C21H40		37	--	3	Value is cetene number x 0.875.
			37	--	4	

Compound	Formula	CAS	CN	Method	Ref.	Comments
2-methyl-2-cyclohexylpentadecane	C22H44		45 45	-- --	3 4	Value is cetene number x 0.875.
1,2,4-trimethyl-5-hexadecylcyclohexane	C25H50		42 42	-- --	3 4	Value is cetene number x 0.875
5-cyclohexyleicosane	C26H52		66 66	-- --	3 4	

6.4 *Olefins*

Compound	Formula	CAS	CN	Method	Ref.	Comments
1-hexene	C6H12	592-41-6	27 27.3	blend delay	1 9	
1-heptyne	C7H12	628-71-7	22	IQT	38	
1-heptene	C7H14	592-76-7	32	IQT	38	
cis-2-heptene	C7H14	14686-13-6	44	blend	1	Cis isomer surmised from boiling point and density data.
vinyl cyclohexane	C8H14	695-12-5	38	--	8	Use ON→CN correlation in Ref 39.
1-octene	C8H16	111-66-0	40.5 41	-- --	5 2	
2,4,4-trimethyl-1-pentene	C8H16	107-39-1	10 11	-- blend	4 1	
2-octene	C8H16	7642-04-8	43	blend	1	
1-nonene	C9H18	124-11-8	50.7 51	-- --	6 2	
2,6-dimethylheptene	C9H18		51	blend	1	
1,9-decadiene	C10H18	1647-16-1	39.8	IQT	38	
1-decene	C10H20	872-05-9	50.2 59 60.2	-- -- --	5 6 2	
1-undecene	C11H22	821-95-4	65 65.5	-- --	6 2	
1-dodecene	C12H24	112-14-4	71 71.3	-- --	2 5	

Compound	Formula	CAS	CN	Method	Ref.	Comments
1-tetradecene	C14H28	1120-36-1	79 79 80.5 80.5 82.7	-- -- -- -- --	3 4 6 2 5	Value is cetene number x 0.875.
2,6,7-trimethyl-2,6-tridecadiene	C16H30		24 24	-- --	3 4	Value is cetene number x 0.875.
1-hexadecene	C16H32	629-73-2	84.2 86.2 87.6 88	-- -- -- --	5 6 2 3	
5-butyl-4-dodecene	C16H32		45 45.5	-- --	3 4	Value is cetene number x 0.875.
2,2,6,6,8,8-hexamethyl-4-methylene-nonane	C16H32	15220-85-6	4.5	--	3	
4-butyl-4-dodecene	C16H32		45	--	11	
7-butyltridecene	C17H34		36 36	-- --	3 4	Value is cetene number x 0.875.
3,12-diethyl-3,11-tetradecadiene	C18H34		26 26	-- --	3 4	Value is cetene number x 0.875
9-methyl-9-heptadecene	C18H36		66 66	-- --	3 4	Value is cetene number x 0.875.
7,10-dimethyl-8-hexadecene	C18H36		43 43	-- --	3 4	Value is cetene number x 0.875.
8-propyl-8-pentadecene	C18H36		45 45	-- --	3 4	Value is cetene number x 0.875

Compound	Formula	CAS	CN	Method	Ref.	Comments
1-octadecene	C18H36	112-88-9	90	--	5	
7-hexyl-7-pentadecene	C21H42		47 47	-- --	3 4	Value is cetene number x 0.875
10,13-dimethyl-11-doeicosene	C24H48		56 56	-- --	3 4	Value is cetene number x 0.875.
4-methyl-1-cyclohexene	C7H12	591-47-9	28 52	-- blend	8 1	Use ON→CN correlation in Ref 39 Value seems anomalous compared to 20–22 for methyl cyclohexane.
4-vinyl-1-cyclohexene	C8H12		32 40	-- blend	8 1	Use ON→CN correlation in Ref 39.

6.5 *Aromatics*

Compound	Formula	CAS	CN	Method	Ref.	Comments
benzene	C6H6	71-43-2	-10 0 14.3 23	-- blend delay blend	3 3 9 1	
toluene	C7H8	108-88-3	-5 9 18.3	blend from ON blend	3 11 1	Use ON→CN correlation in Ref 39. Value is extrapolation of 20, 10, and 5% blends to 0%.
ethyl benzene	C8H10	100-41-4	8	blend	1	
1,2-dimethylbenzene	C8H10	95-47-6	8.3	delay	9	
1,3-dimethylbenzene	C8H10	108-38-3	1	blend	1	
1,4-dimethylbenzene	C8H10	106-42-3	-13	blend	1	
isopropyl benzene	C9H12	98-98-8	15	blend	1	
1,3-diethylbenzene	C10H14	141-93-5	9	blend	1	
sec-butylbenzene	C10H14	135-98-8	6	blend	1	
tert-butyl benzene	C10H14	98-06-8	-1	blend	1	
1,2,3,4-tetramethylbenzene	C10H14	488-23-3	17	blend	1	
1-methyl-4-isopropylbenzene	C10H14	99-87-8	2	blend	1	
n-pentylbenzene	C11H16	538-68-1	8 9 18	-- -- blend	7 3 3	Value is cetene number x 0.875.
biphenyl	C12H10	92-52-4	21 21	-- --	3 7	Value is cetene number x 0.875.

Compound	Formula	CAS	CN	Method	Ref.	Comments
n-hexylbenzene	C12H18	1077-16-3	26 26	-- --	3 2	Value is cetene number x 0.875.
m-diisopropylbenzene	C12H18	99-62-7	-3 -12	-- --	3 3	Value is cetene number x 0.875 Extrapolated from blends.
diphenylmethane	C13H12	101-81-5	11 11	-- --	3 4	Value is cetene number x 0.875
n-propyltetralin	C13H18		8 8	-- --	3 4	Value is cetene number x 0.875.
n-heptylbenzene	C13H20	1078-71-3	34 35 35	-- -- --	3 2 3	 Value is cetene number x 0.875.
1,2-diphenylethane	C14H14	103-29-7	1 1	-- --	3 4	Value is cetene number x 0.875.
?cis-n-butyltetralin ?trans-n-butyltetralin	C14H20		18 18 14	-- -- --	3 4 3	Value is cetene number x 0.875.
sec-butyltetralin	C14H20		7 7	-- --	3 4	Value is cetene number x 0.875.
tert-butyltetralin	C14H20		17 17	-- --	3 4	Value is cetene number x 0.875.
n-octylbenzene	C14H22	2189-60-8	31 32 43	-- -- --	4 3 2	 Value is cetene number x 0.875
2-phenyloctane	C14H22		33 33	-- --	3 4	Value is cetene number x 0.875.

Compound	Formula	CAS	CN	Method	Ref.	Comments
n-nonylbenzene	C15H24	1081-77-2	50 50	-- --	3 4	Value is cetene number x 0.875.
n-octylxylene	C16H26		20 20	-- --	3 4	Value is cetene number x 0.875.
2-phenyl-2-undecene	C17H26		23 23	-- --	3 4	Value is cetene number x 0.875.
2-phenylundecane	C17H28		51 51	-- --	3 4	Value is cetene number x 0.875
n-octyltetralin	C18H28		18 18	-- --	3 4	Value is cetene number x 0.875.
n-dodecylbenzene	C18H30	123-01-3	68 68	-- --	3 4	Value is cetene number x 0.875
4-phenyldodecane	C18H30		42 42	-- --	3 4	Value is cetene number x 0.875.
7-phenyltridecane	C19H32		41 41	-- --	3 4	Value is cetene number x 0.875.
n-tetradecylbenzene	C20H34	1459-10-5	72 72	-- --	3 7	Value is cetene number x 0.875.
2-phenyltetradecane	C20H34		49 49	-- --	3 4	Value is cetene number x 0.875
2-methyl-2-phenylpentadecane	C22H38		39 39	-- --	3 4	Value is cetene number x 0.875.
2-methyl-4-isobutyl-4-phenylundecane	C22H38		18 18	-- --	3 4	Value is cetene number x 0.875.
2-methyl-2-phenylheptadecane	C24H42		39 39	-- --	3 4	Value is cetene number x 0.875.

Compound	Formula	CAS	CN	Method	Ref.	Comments
5-butyl-5-phenyltetradecane	C24H42		58 58	-- --	3 4	Value is cetene number x 0.875. Value of 58 seems anomalously high compared to similar compounds.
1,2,4-trimethyl-5-hexadecylbenzene	C25H44		42 42	-- --	3 4	Value is cetene number x 0.875
di-n-octyltetralin	C26H44		26 26	-- --	3 4	Value is cetene number x 0.875
5-phenyleicosane	C26H46		39 39	-- --	3 4	Value is cetene number x 0.875
tetralin	C10H12	119-64-2	13	blend	1	
1-methylnaphthalene	C11H10	90-12-0	-7 0 0	blend -- --	1 3 7	Primary reference compound.
2,6-dimethylnaphthalene	C12H12	581-42-0	-13	blend	1	
1-n-butylnaphthalene	C14H16	1634-09-9	6 6 6	-- -- --	3 4 7	Value is cetene number x 0.875.
2-(1,1-dimethylethyl)-naphthalene	C14H16	2876-35-9	3 3	-- --	3 4	Value is cetene number x 0.875.
2-methyl-2-(beta-naphthyl)hexane	C17H22		10 10	-- --	3 4	Value is cetene number x 0.875.
2-octylnaphthalene	C18H24	2876-44-0	18 18	-- --	3 4	Value is cetene number x 0.875.
4-methyl-4-(2-naphthyl)heptane	C18H24		9 9	-- --	3 4	Value is cetene number x 0.875

Compound	Formula	CAS	CN	Method	Ref.	Comments
3,6-dimethyl-3-(beta-naphthyl)octane	C20H28		18 18	-- --	3 4	Value is cetene number x 0.875.
5-methyl-5-(beta-naphthyl)nonane	C20H28		12 12	-- --	3 4	Value is cetene number x 0.875
2-methyl-2-(beta-naphthyl)decane	C21H30		18 18	-- --	3 4	Value is cetene number x 0.875
3-ethyl-3-(beta-naphthyl)nonane	C21H30		13 13	-- --	3 4	Value is cetene number x 0.875.

6.6 *Alcohols*

Compound	Formula	CAS	CN	Method	Source	Comments
methanol	CH4O	67-56-1	2 3 3 5	-- -- -- --	37 13 14 15	
ethanol	C2H6O	64-17-5	2 8 11 12	-- -- -- delay	16 13 36 17	
1-propanol	C3H8O	71-23-8	12	--	36	
1-butanol	C4H10O	71-36-3	17	--	36	
1-pentanol	C5H12O	71-41-0	18.2 20	-- --	18 36	
1-hexanol	C6H14O	111-27-3	23.3	--	18	
1-heptanol	C7H16O	111-70-6	28 29.5	IQT --	38 18	
1-octanol	C8H18O	111-87-5	39.1	--	18	
2-ethyl-1-hexanol	C8H18O	104-76-7	23.4	IQT	38	
3-octanol	C8H18O	589-98-0	25.1	IQT	38	
1-nonanol	C9H20O	143-08-8	46.2	--	18	
1-decanol	C10H22O	112-30-1	50.3	--	18	
1-undecanol	C11H24O	112-42-5	53.2	--	18	
1-dodecanol	C12H26O	112-53-8	63.6	--	18	

Compound	Formula	CAS	CN	Method	Source	Comments
1-tetradecanol	C14H30O	112-72-1	51 80.8	delay --	19 18	
palmitoleyl alcohol	C16H32O		46	delay	19	
1-hexadecanol	C16H34O	36653-82-4	68	delay	19	
linolenyl alcohol	C18H32O		41	delay	19	
linoleyl alcohol	C18H34O	506-43-4	44	delay	19	
oleyl alcohol	C18H36O	143-28-2	51	delay	19	
1-octadecanol	C18H38O	112-92-5	81	delay	19	

6.7 Aldehydes/Ketones

Compound	Formula	CAS	CN	Method	Source	Comments
2-heptanone	C7H14O	110-43-0	30	IQT	38	
octanal	C8H16O	124-13-0	80.5	IQT	38	sample contained oxidation inhibitor
3-octanone	C8H16O	106-68-3	35.2	IQT	38	

6.8 Ethers

Compound	Formula	CAS	CN	Method	Source	Comments
dimethyl ether	C2H6O	115-10-6	55 78	-- --	20 21	
dimethoxymethane	C3H8O2	109-87-5	29 49 50 55	-- blend -- --	23 24 25 37	
2-methoxyethanol	C3H8O2	109-86-4	13	--	15	
diethyl ether	C4H10O	60-29-7	140 160	-- delay	37 23	Method not specified.
1,2-dimethoxyethane	C4H10O2	110-71-4	90 98	-- blend	26 26	
1-methoxy-2 propanol	C4H10O2	107-98-2	19	blend	24	
2-butoxyethanol	C6H14O2	111-76-2	35 41	-- blend	27 24	
2-methoxyethyl ether	C6H14O3	111-96-6	>100 109 112-130 126 170 210	-- blend -- -- delay IQT blend	15 28 26 27 23 30	
2,4,7,9-tetra-oxa-decane	C6H14O4		58	blend	24	Because of small difference in blend CN and base fuel CN, blend calculation is not very meaningful.

Compound	Formula	CAS	CN	Method	Source	Comments
hexyl methyl ether	C7H16O	7/3/4747	97	IQT	38	
1-butoxy-2-propanol	C7H16O2	5131-66-8	35.6	IQT	38	
dipropylene glycol monomethyl ether	C7H16O3	34590-94-8	42 44	IQT blend	38 24	
triethylene glycol monomethyl ether	C7H16O4	112-35-6	75	IQT	38	
dibutyl ether	C8H18O	142-96-1	91 100	delay delay	26 26	Delay values are from correlations with reference fuels and with diesel fuels, respectively.
diethoxybutane	C8H18O2		96.6	blend	29	
dimethoxyhexane	C8H18O2		87.6	blend	29	
2-ethoxyethyl ether	C8H18O3	112-36-7	113 133 151	delay delay blend	26 26 24	Delay values are from correlations with reference fuels and with diesel fuels, respectively. Very high CN values not well defined.
dibutoxymethane	C9H20O2	2568-90-3	74 86.6	-- --	25 30	
dipentyl ether	C10H22O	693-65-2	111 130 344	-- blend --	26 26 30	
tripropylene glycol monomethyl ether	C10H22O4	25498-49-1	63 74.5	blend --	24 30	
2-ethoxyethyl acetate	C6H12O3	111-15-9	40	blend	24	

6.9 *Esters*

Compound	Formula	CAS	CN	Method	Source	Comments
methyl sorbate	C7H10O2	689-89-4	6	IQT	38	
ethyl levulinate	C7H12O3	539-88-8	<5	IQT	38	Actual value may be much less than 5.
methyl caproate	C7H14O2	106-70-7	18 24	-- IQT	18 38	
butyl butanoate	C8H16O2	109-21-7	17.8	IQT	38	
methyl heptanoate	C8H16O2	106-73-0	33.5	IQT	38	
glycerol triacetate	C9H14O6	102-76-1	<5	IQT	38	Actual value may be much less than 5.
methyl octanoate	C9H18O2	111-11-5	33.6	--	22	
diethyl adipate	C10H18O4	141-28-6	15	blend	24	
decanoic acid	C10H20O2	334-48-5	47.6	blend	31	Value is from double blend procedure with potential for large errors.
methyl decanoate	C11H22O2	110-42-9	47.2 47.9	-- --	31 18	
dibutyl maleate	C12H20O4	105-76-0	26.5 29	delay blend	30 24	
butyl octanoate	C12H24O2	589-75-3	39.6	--	31	
ethyl decanoate	C12H24O2	110-38-3	51.2 60	-- blend	31 32	
decyl acetate	C12H24O2	112-17-4	62	blend	32	

Compound	Formula	CAS	CN	Method	Source	Comments
methyl laurate	C13H26O2	111-82-0	54 60.8 61.2 61.4 70	delay -- -- -- blend	24 18 12 31 32	
isopropyl decanoate	C13H26O2	2311-59-3	46.6	--	31	
propyl decanoate	C13H26O2	30673-60-0	52.9 64	-- blend	31 32	
octyl valerate	C13H26O2	5451-85-4	49	blend	32	
butyl decanoate	C14H28O2		54.6 63	-- blend	31 32	
acetic acid, dodecyl ester	C14H28O2	112-66-3	77 77	blend blend	32 24	
ethyl laurate	C14H28O2	106-33-2	73	blend	32	
tributyrin	C15H26O6	60-01-5	-5 6.7 40	blend delay blend	24 30 30	
methyl myristate	C15H30O2	124-10-7	66.2 72 73.5	-- blend --	31 32 18	
decyl valerate	C15H30O2		61	blend	32	
propyl laurate	C15H30O2	3681-78-5	71	blend	32	
ethyl myristate	C16H32O2	124-06-1	66.9 72	-- blend	31 32	

Compound	Formula	CAS	CN	Method	Source	Comments
tetradecyl acetate	C16H32O2		81	blend	32	
hexyl caprate	C16H32O2		64	blend	32	
butyl laurate	C16H32O2		73	blend	32	
palmitoleic acid, methyl ester	C17H32O2		51	delay	33	
methyl palmitate	C17H34O2	112-39-0	74.3 74.5 80 85.6 91	D 613 D 613 BASF IQT delay	18 31 32 33 19	
dodecyl valerate	C17H34O2		67	blend	32	
propyl myristate	C17H34O2		71	blend	32	
linolenic acid	C18H30O2	463-40-1	20.4	delay	34	
linoleic acid	C18H32O2	60-33-3	31.4	delay	34	
oleic acid	C18H34O2	112-80-1	46.1	delay	34	
butyl myristate	C18H36O2		69.4 73	-- blend	31 32	
hexadecyl acetate	C18H36O2	629-70-9	86	blend	32	
hexyl laurate	C18H36O2		74	blend	32	
ethyl palmitate	C18H36O2	628-97-7	80 93.1	blend delay	32 33	
stearic acid	C18H36O2	57-11-4	61.7	delay	34	
linolenic acid, methyl ester	C19H32O2		22.7	delay	34	

Compound	Formula	CAS	CN	Method	Source	Comments
methyl linoleate	C19H34O2	112-63-0	38.2	delay	33	
			41.7	--	12	
			42.2	delay	34	
			42.6	--	22	
			45.9	--	12	
methyl oleate	C19H36O2	112-62-9	52.5	--	22	
			55	delay	34	
			56.0	--	12	
			59.3	delay	33	
			71	blend	32	
			80	delay	19	
methyl stearate	C19H38O2	112-61-8	75.6	D 613	18	
			81	IQT	33	
			86.9	blend	31	
			100	delay	19	
			101	BSAF	32	
tetradecyl valerate	C19H38O2		68	blend	32	
propyl palmitate	C19H38O2		83	blend	32	
			85	delay	33	
isopropyl palmitate	C19H38O2	142-91-6	82.6	delay	33	
linolenic acid, ethyl ester	C20H34O2		26.7	delay	34	
linoleic acid, ethyl ester	C20H36O2	544-35-4	37.1	delay	34	
			39.6	delay	33	
			44.4	--	12	

Compound	Formula	CAS	CN	Method	Source	Comments
ethyl oleate	C20H38O2	111-62-6	53.9 67.8 72	delay delay blend	34 33 32	
octadecyl acetate	C20H40O2	822-23-1	90	blend	32	
decyl caprate	C20H40O2	1654-86-0	81	blend	32	
octyl laurate	C20H40O2		84	blend	32	
hexyl myristate	C20H40O2		72	blend	32	
butyl palmitate	C20H40O2	111-06-8	87 91.9	blend delay	32 33	
ethyl stearate	C20H40O2	111-61-5	76.8 86 97.7	delay blend delay	34 32 33	
isobutyl palmitate	C20H40O2		83.6	delay	33	
2-butyl palmitate	C20H40O2		84.8	delay	33	
linolenic acid, propyl ester	C21H36O2		26.8	delay	34	
linoleic acid, propyl ester	C21H38O2		40.6 44	delay delay	34 33	
propyl oleate	C21H40O2		58.8 72	delay blend	33 32	
isopropyl oleate	C21H40O2		86.6	delay	33	
oleic acid, propyl ester	C21H40O2		55.7	delay	34	
hexadecyl valerate	C21H42O2		70	blend	32	
methyl arachidate	C21H42O2		100	delay	19	
propyl stearate	C21H42O2	3634-92-2	69.9 90.9	delay delay	34 33	

Compound	Formula	CAS	CN	Method	Source	Comments
isopropyl stearate	C21H42O2		96.5	delay	33	
linolenic acid, butyl ester	C22H38O2		28.6	delay	34	
linoleic acid, butyl ester	C22H40O2		41.6 53.5	delay delay	34 33	
butyl oleate	C22H42O2	142-77-8	59.8 61.6 102	delay delay blend	34 35 32	
isobutyl oleate	C22H42O2		59.6	delay	33	
2-butyl oleate	C22H42O2	142-77-8	71.9	delay	33	
decyl laurate	C22H44O2		84	blend	32	
octyl myristate	C22H44O2		71	blend	32	
hexyl palmitate	C22H44O2		87	blend	32	
butyl stearate	C22H44O2	123-95-5	80.1 92.5	delay delay	34 33	
isobutyl stearate	C22H44O2		99.3	delay	33	
2-butyl stearate	C22H44O2		97.5	delay	33	
hexyl oleate	C24H46O2		102	blend	32	
dodecyl laurate	C24H48O2		85	blend	32	
2-ethylhexyl palmitate	C24H48O2		98.2	delay	33	
decyl myristate	C24H48O2		72	blend	32	
octyl palmitate	C24H48O2		107	blend	32	
octyl oleate	C26H50O2		131	blend	32	
2-ethylhexyl oleate	C26H50O2		88.2	delay	33	
dodecyl myristate	C26H52O2		74	blend	32	
decyl palmitate	C26H52O2		91	blend	32	
2-ethylhexyl stearate	C26H52O2		115.5	delay	33	

Compound	Formula	CAS	CN	Method	Source	Comments
hexadecyl laurate	C28H56O2		88	blend	32	
dodecyl oleate	C30H58O2		134	blend	32	
trilaurin	C39H74O6		100	delay	19	
trimyristin	C45H86O6		100	delay	19	
tripalmitin	C51H98O6		89	delay	19	
trilinolenin	C57H92O6		23	delay	19	
trilinolein	C57H98O6		32	delay	19	
triolein	C57H104O6		45	delay	19	
tristearin	C57H110O6		85	delay	19	

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