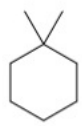
ISOMERS

Structural (Constitutional) Isomers

- Share the same molecular formula but have the atomic bonds in different places

Example 1



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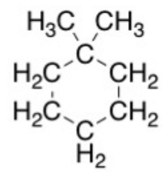
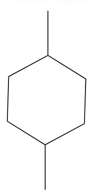


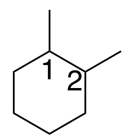
C_8H_{16}

1,1-dimethylcyclohexane



C_8H_{16}

1,4-dimethylcyclohexane

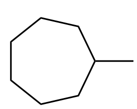


1,2-dimethylcyclohexane

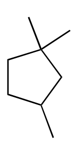
The above three compounds are structural (also known as constitutional) isomers

Example 2

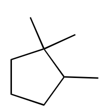
Structural or constitutional isomers



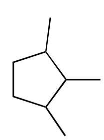
1-methylcycloheptane



1,1,3-trimethylcyclopentane



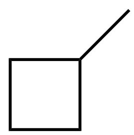
1,1,2-trimethylcyclopentane



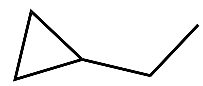
1,2,3-trimethylcyclopentae

Example 3

C_5H_{10}
structural isomers



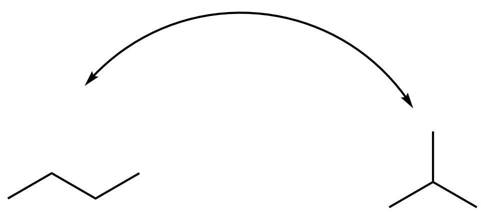
1-methylcyclobutane



1-ethylcyclopropane

Example 4

structural isomers



n-butane

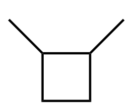
C_4H_{10}

2-methylpropane

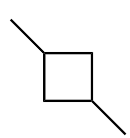
C_4H_{10}

Example 5

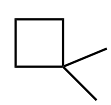
Structural or constitutional isomers



1,2-dimethylcyclobutane



1,3-dimethylcyclobutane



1,1-dimethylcyclobutane

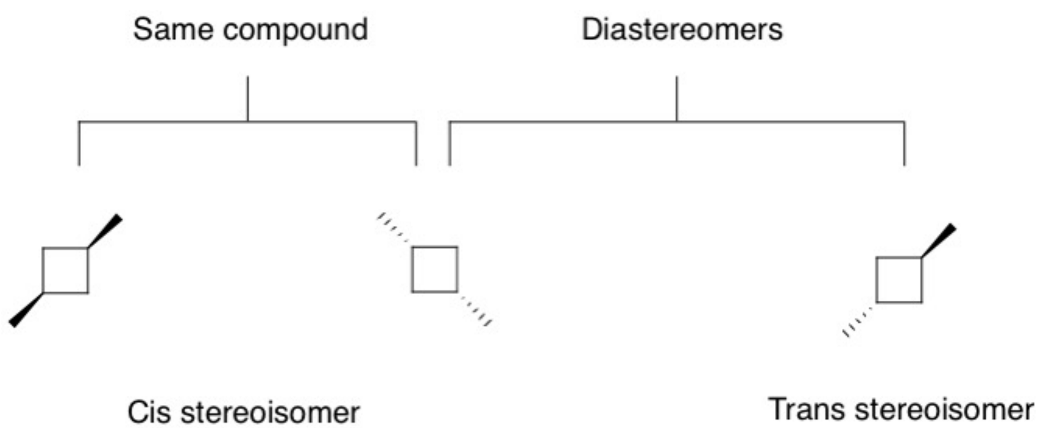
Stereoisomers

Compounds with the same molecular formula, same order of connection (base name) but connection of atoms that differ in 3D geometry

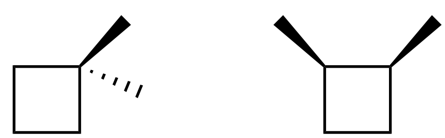
Two Types:

1. Diastereomers - stereoisomers that are not mirror images (all stereoisomers that are not enantiomers)
2. Enantiomers - stereoisomers that are non-superimposable mirror images of each other

Example: 1,3-dimethylcyclobutane



Structural Isomers:

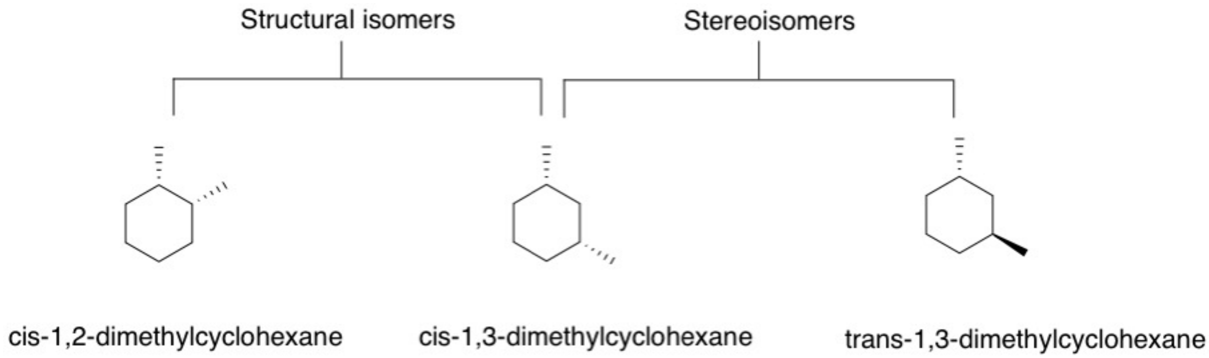


The first and second compounds are the same compound rotated in 3D space. The third compound has different geometry at one center, making it a stereoisomer, specifically a diastereomer.

Cis - the substituents are on the same side of the ring

Trans - the substituents are on opposite sides of the ring

Example: 1,2-dimethylcyclohexane and 1,3-dimethylcyclohexane

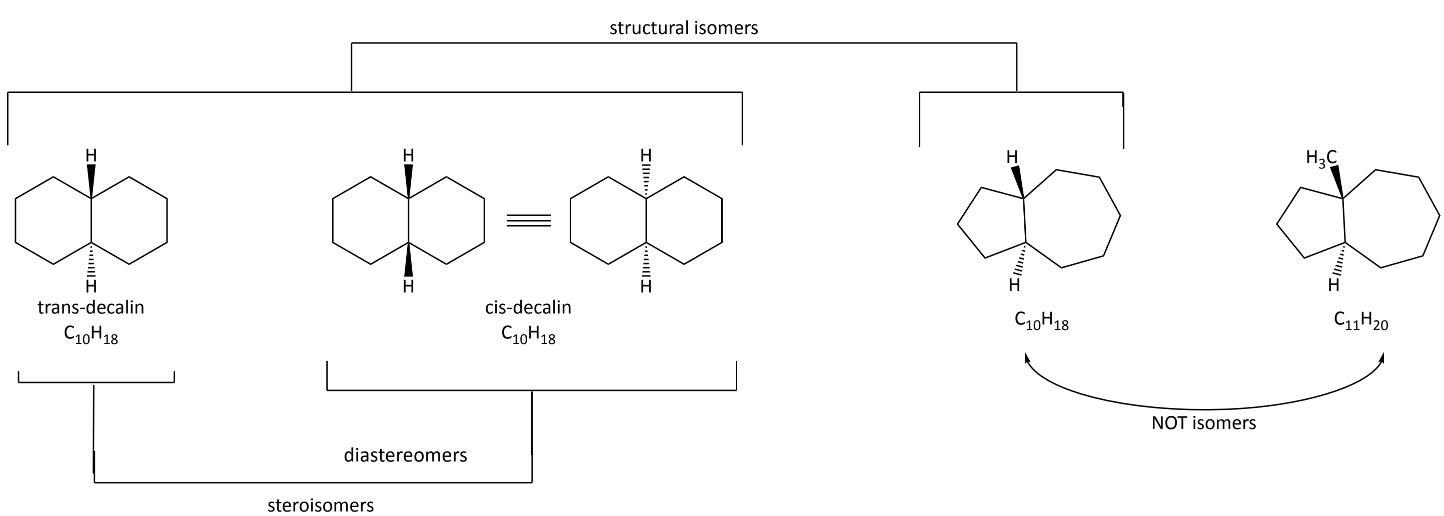


The second two compounds are diastereomers of each other.

Example: Are these compounds structural isomer of each other?

These compounds are not structural isomer of each other because they have different molecular formula

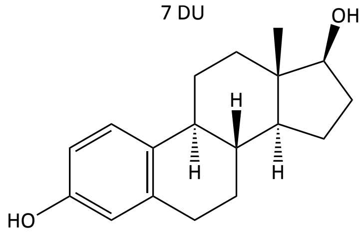
Example: decalin - $C_{10}H_{18}$



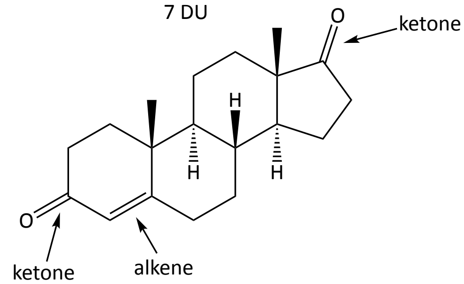
Example: steroids

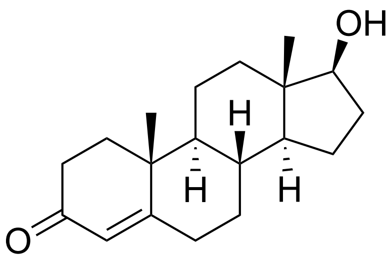
androstenedione

estradiol
7 DU



testosterone
7 DU

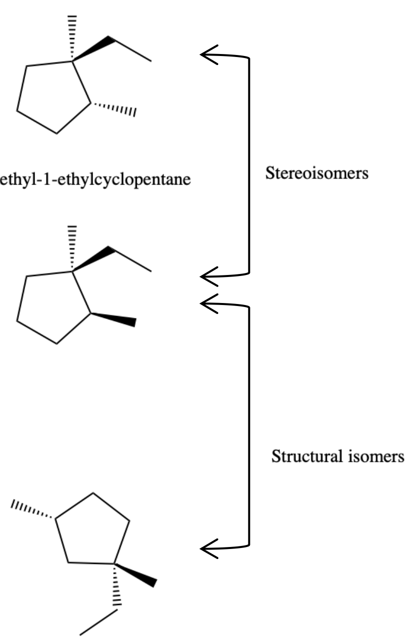




Testosterone
Molecular formula?
Functional groups?
Degrees of Unsaturation?
How many methyls?
How many methylenes?
How many methines?

TEST YOURSELF

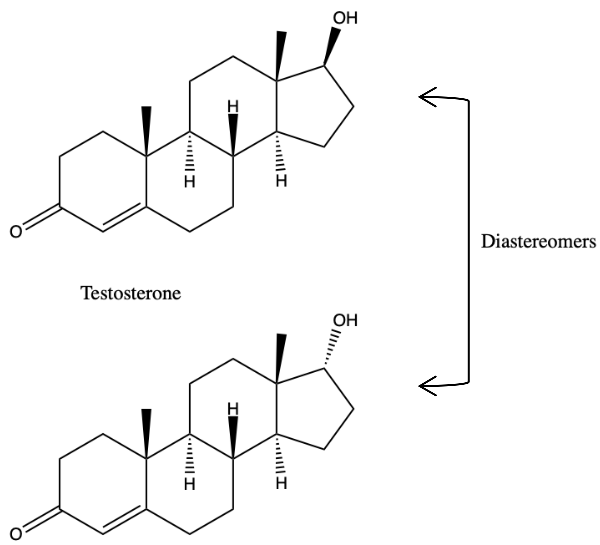
Example:



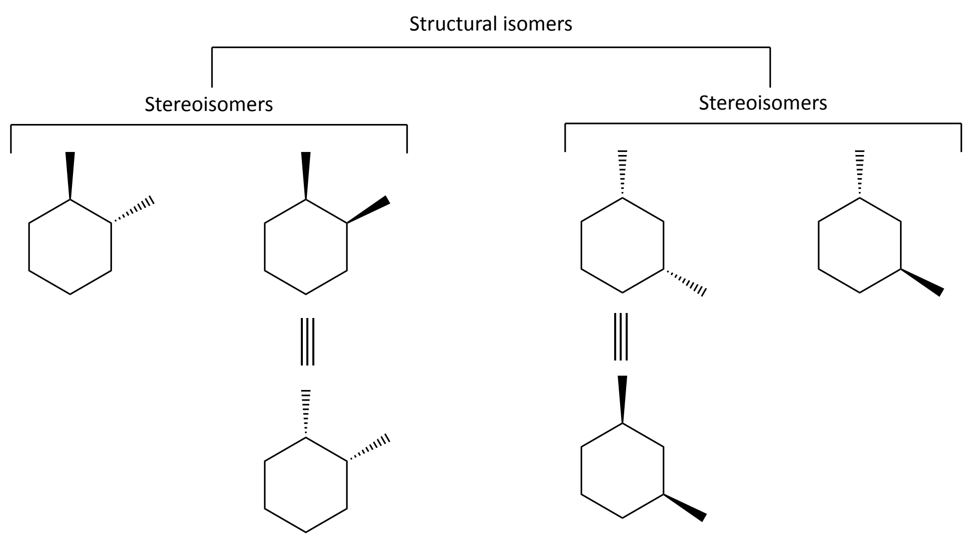
1,2-Dimethyl-1-ethylcyclopentane

1,3-Dimethyl-1-ethylcyclopentane

Example of diastereomers:

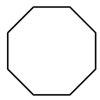


<u>More on differentiating structural and stereoisomers</u>

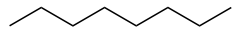


trans-1,2-dimethylcyclohexane | cis-1,2-dimethylcyclohexane | cis-1,3-dimethylcyclohexane | trans-1,3-dimethylcyclohexane

Example:



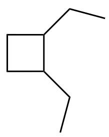
cyclooctane
C_8H_{16}
DOU = 1



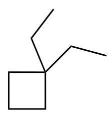
n-octane
C_8H_{18}
DOU = 0

Cyclooctane and 1,2-diethylcyclobutane and 1,1-diethylcyclobutane are structural (constitutional) isomers – they all have the same molecular formula

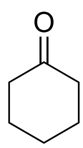
n-octane is not a structural isomer of the others, it has a different molecular formula



1,2-diethylcyclobutane
C_8H_{16}
DOU = 1



1,1-diethylcyclobutane
C_8H_{16}
DOU = 1



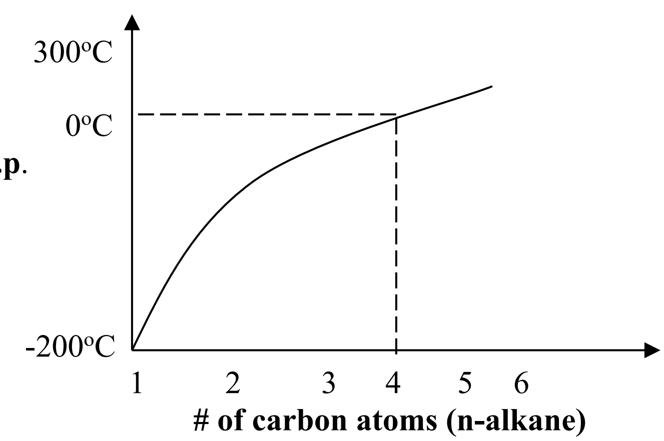
Degrees of Unsaturation = 2
(1 ring and 1 double bond)
$C_6H_{10}O$

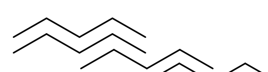
<u>Physical Properties of Alkanes:</u>

Boiling Point

Intermolecular forces are dominated by London forces

- Alkanes are non-polar because H and C have similar electronegativity leading them to interact with themselves through London Forces which causes a trend in boiling point:



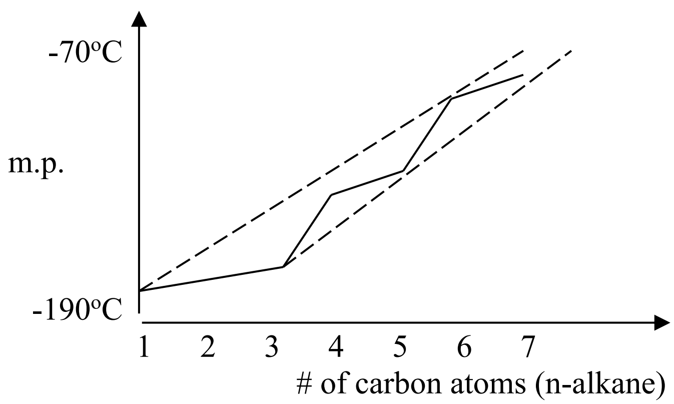


London Forces (temporary dipoles) hold molecules together

The boiling point increases as the size of the alkane increases because the longer carbon chains have greater surface area to experience London Forces. As the boiling point increases, the graph reaches a plateau where alkane starts to decompose (#C > 20)

Melting point

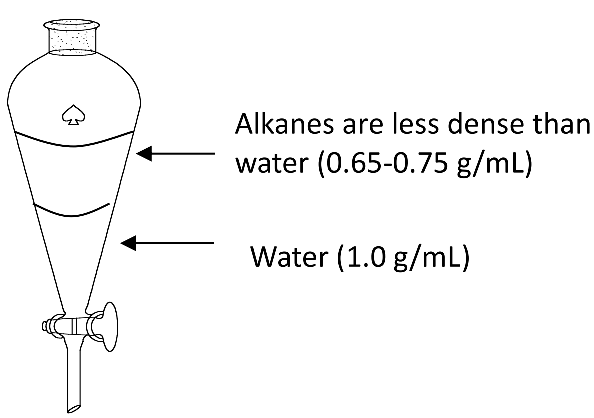
- Melting points are related to the crystal structure packing efficiency
- The predicted line (dotted line) is not what we observe, but a zig zag line (continuous) resulting from crystal structure packing.
- Even numbered alkanes pack better in a crystal lattice
- Alkanes are flammable and will combust into CO_2 and H_2O



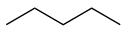
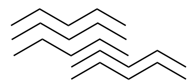
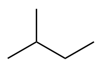
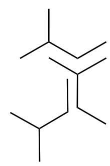
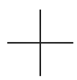
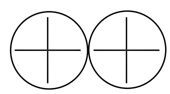
Solubility

- Alkanes are soluble in other organic solvents (like dissolves like)
- Not miscible (soluble) with water → floats due to lower density
- Low density (ρ = rho = g/cm^3)
    - ρ water ~ 1 g/cm^3 or 1 g/mL
    - ρ alkanes ~ 0.7 g/cm^3

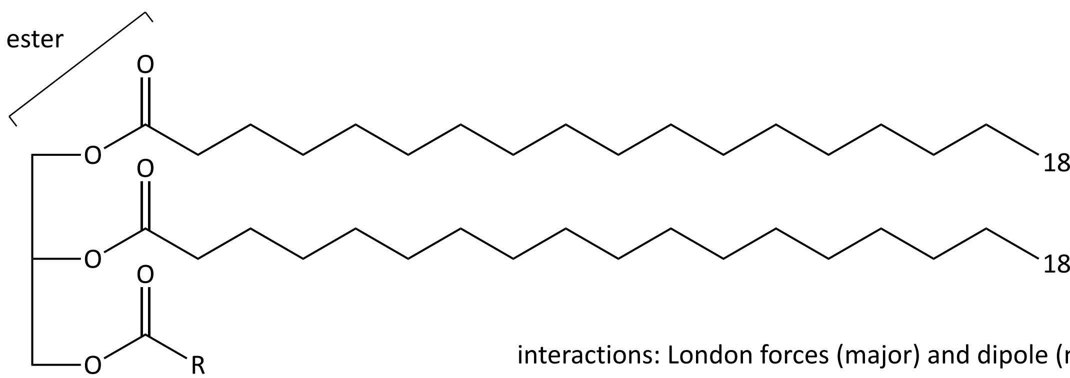
Separatory Funnel *(density separation)*



Example: Pentane

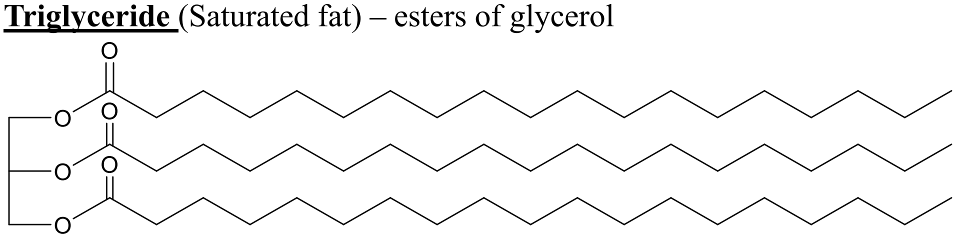
	m.p.	b.p.		
 **n-pentane**	-129	36		n-pentane has high bp due to multiple contacts of straight chains (London Forces)
 **isopentane** **2-methylbutane**	-160	28		isopentane is less well packed, less interacting surface area
 **neopentane** **2,2-dimethylpropane**	-13	9		m.p. of neopentane determined by good crystal packing of spherical shape. Ball-like shape means surface contact area small and boiling point lower

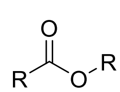
E.g.



interactions: London forces (major) and dipole (min)

Triglyceride (Saturated fat) – esters of glycerol



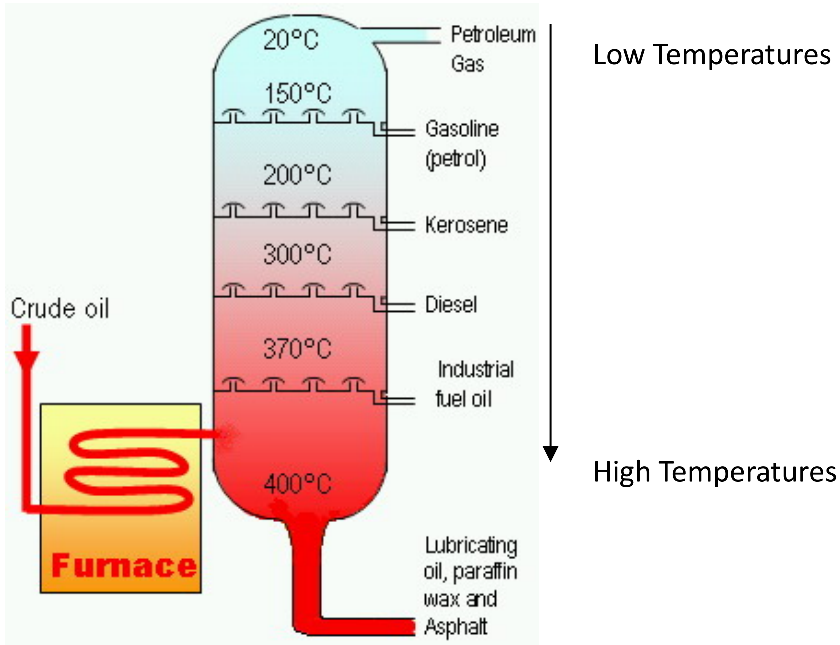
Ester Group = 

Molecules are held predominantly by London Forces. Some dipole-dipole interactions can occur due to the ester groups present.

<u>Source of Alkanes</u>

- Petroleum

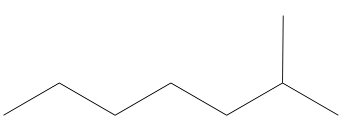
Distillation of Petroleum:



- Petroleum is a mixture of alkanes and other hydrocarbons (>>200 compounds)

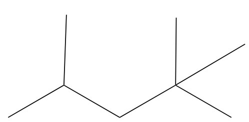
Fuel (gasoline)

A fuel composed of 100% "isooctane" (incorrect name) will have an octane rating of 100. 2,2,4-trimethylpentane "isooctane" is the best burning. Heptane is the worst burning (explosive burning). A fuel that burns like a mixture of 90:10 "isooctane" to heptane has a 90 octane rating.



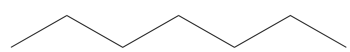
isooctane

2-methylheptane



incorrectly also called "isooctane"

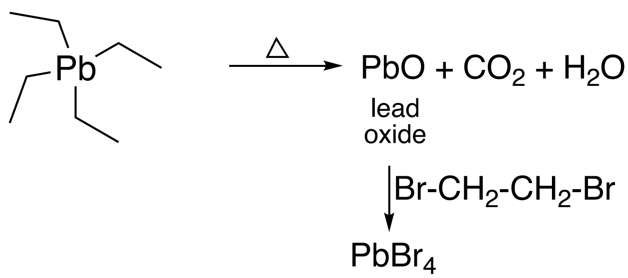
2,2,4-trimethylpentane



heptane

At the pump you typically see an octane rating between 88 and 94.

Tetramethyl Lead
-highly toxic



Volatile and highly toxic