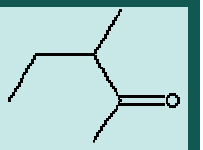
METHYL ISOBUTYL KETONE

PRODUCT IDENTIFICATION



CAS NO	108-10-1
EINECS NO.	203-550-1
FORMULA	$(CH_3)_2CHCH_2COCH_3$
MOL WT.	100.16
H.S. CODE	2914.13
TOXICITY	Oral rat LD50; 2737 mg/kg
SYNONYMS	MIBK; Isopropylacetone; 4-Methyl-2-pentanone; 2-methyl-4-pentanone; 4-Methylpentan-2-one; Hexanone; Hexone; Isohexanone; Isopropylacetone;
DERIVATION	
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES

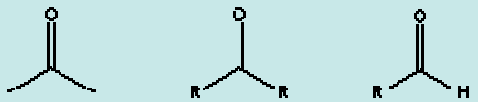
PHYSICAL STATE	Clear, volatile liquid, mild acetone odor
MELTING POINT	-85 C
BOILING POINT	114 - 117 C
SPECIFIC GRAVITY	0.799 - 0.802
SOLUBILITY IN WATER	Soluble
pH	
VAPOR DENSITY	
AUTOIGNITION	400 C
NFPA RATINGS	Health: 1; Flammability: 3; Reactivity: 0
REFRACTIVE INDEX	1.3962
FLASH POINT	14 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION and APPLICATIONS

Ketone is a class of chemical compounds contain the carbonyl group in which the carbon atom is covalently bonded to an oxygen atom.

Carbonyl groups are:

- Aldehydes (X and Y = H; X = H, Y = alkyl or aryl)
- Ketones (X and Y = alkyl or aryl)
- Carboxylic acids (X = OH, Y = H, alkyl, or aryl)
- Esters (X = O-alkyl or aryl; Y = H, alkyl, or aryl)
- Amides (X = NH, N-alkyl, or N-aryl; Y = H, alkyl, or aryl)
- Acid halides
- Acid anhydrides
- Lactones
- Lactams



Carbonyl Group Ketones Aldehydes

Ketone has the general formula RCOR' where the groups R and R' may be the same or different, or incorporated into a ring (R and R' are alkyl, aryl, or heterocyclic radicals). The simplest example, R and R´ are methyl group, is acetone (also called 2-propanone, CH_3COCH_3) which is one of the most important ketones used in industry (low molecular weight ketones are general purpose solvents.) In the IUPAC system, the suffix -one is used to describe ketone with the numbering of the carbon atom at the end that gives the lower number. For example, $CH_3CH_2COCH_2CH_2CH_3$ is named 3-hexanone because the whole chain contains six carbon atoms and the oxygen is connected to the third carbon from the lower number. There are aromatic ketones of which acetophenone and bezophenone are examples. Ketones can be made by the oxidation of secondary alcohols and the destructive distillation of certain salts of organic acids. In addition to as polar solvents, ketones are important intermediates in the syntheses of organic compounds such as alkoxides, hydroxyalkynes, imines, alcohols (primary, secondary as well as tertiary), acetals, thioacetals, phosphine oxides, geminal diols, hydrazones, organic sulfite and cyanohydrins.

Methyl Isobutyl Ketone (MIBK) is a clear liquid with a mild characteristic odor; miscible in oil, soluble in water.

MIBK is a polar solvent. But the polarity is similar to ethyl acetate. Water solubility is not good compare to other ketone solvents like acetone and MEK (methyl ethyl ketone). This property makes MIBK an useful liquid-liquid extraction solvent. MIBK is produced from acetone with hydrogen by three-step process (aldol condensation, dehydration, hydrogenation). Aiacetone alcohol (CAS #: 123-42-2) and mesityl oxide (CAS #: 141-79-7) are intermediate products during the process. The basic unit quantity of acetone to produce 1 unit of MIBK is 1.22. MIBK has good compatibility with various organic reagents and solvency power for a variety industrial materials. It is primarily used in cellulose-based and resin-based coatings and adhesives. It is also employed in rare-metal extraction. It is used in dewaxing to purify pharmaceuticals, mineral oils, fatty acids, and alcohols. MIBK is also an useful intermediate to produce target molecules, rubber antiozonants (e.g. 6PPD) and acetylenic diol compounds are examples of end products.

Diacetone alcohol has slow evaporation rates. It is used as a solvent for both hydrogen bonding and polar substances. It is miscible in water and used as a solvent for water-based coatings. It is used as a solvent extractant in purification processes for resins and waxes. Diacetone alcohol is more suitable for use in applications as a component of gravure printing inks, with proving favorable flow and leveling characteristics. Diacetone alcohol, having hydroxyl and carbonyl group in the same molecule is used as a chemical intermediate.

Mesityl oxide, a carbonyl compound having alpha (or beta) unsaturated chain, can be used as a raw material to produce drugs, solvents and plasticizer. Mesityl oxide is used to produce hydroperoxides. Mesityl oxide is as an extractant in ore flotation especially for actinide series elements (thorium and uranium).

Diisobutyl Ketone, having the higher boiling than MIBK, is produced by refining heavy end from MIBK. DIBK has moderate solvent activity for polymers including nitrocellulse, alkyd, vinyl and epoxy resins. DIBK is a component for solvents in sealants and inks. It is used as an extraction solvent and as an aid to purify pharmaceuticals.

SALES SPECIFICATION	
APPEARANCE	Clear liquid
PURITY	99.5% min
COLOR. APHA	10 max
WATER	0.05% max
NONVOLATILES	0.002% max
DISTILLATION RANGE	114 - 117 C

TRANSPORTATION	
PACKING	160kgs in drum
HAZARD CLASS	3 (Packing Group: III)
UN NO.	1245

OTHER INFORMATION

European Hazard Symbols: F XI, Risk Phrases: 11-20-36/37-66, Safety Phrases: 9-16-29

GENERAL DESCRIPTION OF SOLVENT

Solvent is a substance, usually a liquid, that acts as a dissolving agent or that is capable of dissolving another substance. In solutions of solids or gases in a liquid, the liquid is the solvent. In all other homogeneous mixtures (i.e., liquids, solids, or gases dissolved in liquids; solids in solids; and gases in gases), solvent is the component of the greatest amount. The minor proportion substances are called solutes. The solvent offers several functions during a chemical reaction. It solves not only the substance that reacts with another one to produce a new set of substances (reactant) but also the compound that supplies the molecule, ion, or free radical, which is considered as the attacking species in a chemical reaction (reagent). The solvent is conductive to collisions between the reactants and reagents to transform the reactants to new products. The solvent also takes roll of temperature control, either to provide the energy of the colliding particles for speedy reaction and to absorb heat in exothermic reaction. The appropriate solvent should be selected based on the inactivity in the reaction conditions, dissolving the reagents as well as reactants, appropriate boiling point and easy removal at the end of the reaction.

Polarity

The most common solvent is water. Other common solvents which dissolve substances that are insoluble (or nearly insoluble) in water are acetone, alcohol, formic acid, acetic acid, formamide. BTX, carbon disulfide, diemthyl sulfoxide, carbon tetrachloride, chloroform, ether, tetrahydrofuran, furfural, hexane and turpentine. They may be classified as polar and non-polar. Polar solvents, like water, have molecules whose electric charges are unequally distributed, leaving one end of each molecule more positive than the other. Usually polar solvent has O-H bond of which water (HOH), (CH_3OH) and acetic acid (CH_3COOH) are examples. Propanol, butanol, formic acid, formamide are polar solvents. Dipolar solvents which contain a C-O solid bond without O-H bond are acetone [$(CH_3)_2C=O$], ethyl acetate ($CH_3COOCH_2CH_3$), methyl ethyl ketone, acetonitrile, N,N-dimethylformamide and diemthyl sulfoxide. Nonpolar solvents, like carbon tetrachloride

(CCl_4), benzene (C_6H_6), and diethyl ether ($CH_3CH_2OCH_2CH_3$), have molecules whose electric charges are equally distributed and are not miscible with water. Hexane, tetrahydrofuran and methylene chloride are non-polar solvents. Polar solvents are hydrophilic but non-polar solvents are lipophilic. Polar reactants will dissolve in polar solvents. Non-polar solvents dissolve non-polar compounds best. Oil and water don't mix but separate into two layers. There are three measures of the polarity as "dipole moment", "dielectric constant" and "miscibility with water". Though low dipole moments and small dielectric constants indicates non-polar solvents, sharp boundaries between polar and non-polar solvents are not available. The polarity reflects the balance between a polar component (OH) and a non-polar hydrocarbon component, existing in the same molecule. If hydrocarbon character increases relatively, the polarity decreases. On an operational basis, solvents that are miscible with water are polar.

Polar Protic and Dipolar Aprotic

Protic refers to a hydrogen atom attached to an electronegative atom. Protic solvents can donate an H+ (proton) since they contain dissociable H+, such as hydrogen attached to oxygen as in a hydroxyl group, nitrogen as in a amine group. Examples are water, methanol, ethanol, formic acid, hydrogen fluoride and ammonia. Aprotic solvents don't has O-H bond but a C=O bond typically. Examples are acetone [$(CH_3)_2C=O$] and ethyl acetate ($CH_3COOCH_2CH_3$). Polar protic solvents are useful in S_N1 reaction, while polar aprotic solvents are S_N2 reaction.

Solvents	Boiling point C	Dipole Moment	Dielectric Constant	Density (g/ml)
Polar Protic				
Water	100	1.85	80	0.998
Methanol	68	1.70	33	0.791
Ethanol	78	1.69	24.3	0.789
n-Propanol	97	1.68	20.1	0.803
n-Butanol	118	1.66	17.8	0.810
Formic acid	100	1.41	58	1.21
Acetic acid	118	1.74	6.15	1.049
Formamide	210	3.73	109	1.134
Polar Aprotic				
Acetone	56	2.88	20.7	0.786
Tetrahydrofuran	66	1.63	7.52	0.886
Methyl ethyl ketone	80	2.78	18.5	0.805
Ethyl acetate	78	1.78	6.02	0.894
Acetonitrile	81	3.92	36.6	0.786
N,N-Dimethylformamide	153	3.82	38.3	0.944
Diemthyl sulfoxide	189	3.96	47.2	1.092
Non-Polar				
Hexane	69	-	2.02	0.655
Benzene	80	0	2.28	0.879
Diethyl ether	35	1.15	4.34	0.713
Methylene chloride	40	1.60	9.08	1.326
Carbon tetrachloride	76	0	2.24	1.594