ACETONE

IUPAC name: Propanone
Other Names: β-ketopropane, Dimethyl ketone, dimethylformaldehyde, DMK
CAS: 67-64-1
RTECS Number: AL31500000
Molecular Formula: CH_3COCH_3
Molar Mass: 58.08 g/mol
Appearance: Colorless liquid
Density: 0.79 g/cm³, liquid
Melting Point: −94.9 °C (178.2 K)
Boiling Point: 56.53 °C
Solubility in Water: miscible
Viscosity: 0.32 cP at 20 °C
Molecular Shape: trigonal planar at C=O
Dipole Moment: 2.91 D
Hazards EU Classification: F, Xi
R-phrases: R11, R36, R66, R67
S-phrases: (S2), S9, S16, S26
Flash Point: -17 °C
Autoignition Temperature: 465 °C
Spectral Data: UV, IR, NMR, MS

Except where noted otherwise, data are given for materials
in their standard state at 25 °C, 100 kPa

Acetone (also known as propanone, dimethyl ketone, 2-propanone, propan-2-one, dimethylformaldehyde and β-ketopropane) is colorless, mobile, flammable liquid. It is the simplest example of ketones. Miscible with water, ethanol, ether and itself serves as an important solvent. The most familiar household uses of acetone are as the active ingredient in nail polish remover and to thin some paints. Acetone is used to make plastic, fibers, drugs, and other chemicals. In addition to being manufactured as a chemical, acetone is found naturally in the environment, including in small amounts in the human body.

Production
Acetone is produced primarily in the cumene process. Previously, acetone was produced by the dry distillation of acetates, for example calcium acetate. During WWI a new process of producing acetone through bacterial fermentation was developed by Chaim Weizmann in order to help the British war effort. This Acetone Butanol Ethanol process was abandoned due to the small yield of Acetone Butanol compared to the organic waste.

Biosynthesis
See also: ketosis
The body produces small amounts of acetone by decarboxylation of ketone bodies.

Uses
Cleaning fluid
Acetone is also used as a superglue remover. It can be used for thinning and cleaning fiberglass resins and epoxies. Strong solvent for most plastics and synthetic fibres. Ideal for thinning fiberglass resin, cleaning fiberglass tools and dissolving two-part epoxies and superglue before hardening. Heavy-duty degreaser, it is useful in the preparation of metal prior to painting; it thins polyester resins, vinyl and adhesives. It easily removes residues from glass and porcelain. In biological research contexts, buffers that contain acetone (as citrate-buffered formalin) use the acetone to lyse cells for further experimentation. Acetone is effectively used as cleaning agent when dealing with permanent markers.

Solvent

Acetone can also dissolve many plastics, including those used in Nalgene bottles made of polystyrene, polycarbonate and some types of polypropylene.
In laboratory, acetone is used as polar aprotic solvent in variety of organic reactions, such as S_N2 reactions.
The use of acetone solvent is also critical for the successful Jones oxidation.
Technical grade acetone is inexpensive. Because of acetone's medium polarity, it dissolves a wide range of compounds. Thus, it is commonly loaded into squeeze bottles and used as a general solvent in rinsing laboratory glassware.
Though flammable itself, acetone is also used extensively for the safe transporting and storing of acetylene in the mining industry. Vessels containing a porous material are first filled with acetone followed by acetylene, which dissolves into the acetone. One liter of acetone can dissolve around 250 liters of acetylene.

Feedstock

Important industrial use for acetone involves its reaction with phenol for manufacture of bisphenol A. Bisphenol A is an important component of many polymers such as polycarbonates, polyurethanes and epoxy resins.
Acetone has also been used in the manufacture of cordite.

Other uses

Drying agent, due to the readiness with which it mixes with water, and its volatility.
It can be used as an artistic agent; when rubbed on the back of a laser print or photocopy placed face-down on another surface and burnished firmly, the toner of the image is allowed to transfer to the destination surface.
Acetone can be cooled with dry ice to -78 °C without freezing; acetone/dry ice baths are commonly used to conduct reactions at low temperatures.
Acetone is fluorescent under ultraviolet light, and acetone vapor may be used as a fluorescent tracer in fluid flow experiments.

Safety

Flammability

Most common hazard associated with acetone is extreme flammability.
It auto-ignites at temp 465 °C. At temp greater than acetone's flash point of -20 °C, air mixtures of 2.5 - 12.8% acetone, by volume, may explode or cause a flash fire.
Vapors can flow along surfaces to distant ignition sources and flash back.
Static discharge may also ignite acetone vapors.

Acetone peroxide

Oxidized, acetone forms acetone peroxide as by-product, highly unstable compound. It may be formed accidentally, e.g. when waste hydrogen peroxide is poured into waste solvent containing acetone.
Acetone peroxide is >10 times as friction and shock sensitive as nitroglycerin.
Due to its instability, it is rarely used, despite its easy chemical synthesis.

Toxicology

Acetone is believed to exhibit only slight toxicity in normal use, and there is no strong evidence of chronic health effects if basic precautions are followed.
At very high vapor concentrations, acetone is irritating and, like many other solvents, may depress central nervous system. It is also a severe irritant on contact with eyes, and a potential pulmonary aspiration risk. In one documented case, ingestion of a substantial amount of acetone led to systemic toxicity, although the patient eventually fully recovered. Some sources estimate LD_{50} for human ingestion at 1.159 g/kg; LD50 inhalation by mice is given as 44g per cubic meter, over 4 hours.
Interestingly, acetone has been shown to have anticonvulsant effects in animal models of epilepsy, in absence of toxicity, administered in millimolar concentrations. It has been hypothesized that high fat low carbohydrate ketogenic diet used clinically to control drug-resistant epilepsy in children works by elevating acetone in the brain.

Environmental Effects
Acetone evaporates rapidly, even from water and soil.
Once in atmosphere, it is degraded by UV light with 22-day half-life.
Acetone dissipates slowly in soil, animals, or waterways since it is sometimes consumed by microorganisms; it is significant issue with respect to groundwater contamination due to high solubility in water.
LD_{50} of acetone for fish is 8.3g/l of water (or about 0.8%) over 96 hours, and its environmental half-life is about 1 to 10 days. Acetone may pose a significant risk of oxygen depletion in aquatic systems due to the microbial activity consuming it.
CERCLA requires reporting a spill of 5000 lbs or more.
Acetone is included in the 40CFR51.100 list as VOC exempt.
http://www.cdpr.ca.gov/docs/emon/vocs/vocproj/2voc_exempt_list.pdf

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