CYCLOHEXANONE (CYC)

Chemical Formula: C₆H₁₀O

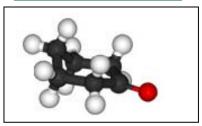
CAS Registry Number: 108-94-1

Molecular Weight: 98.14

Category: Ketone

NOTICE: THE INFORMATION BELOW IS BELIEVED TO BE ACCURATE AND REPRESENTS THE BEST INFORMATION CURRENTLY AVAILABLE TO US. HOWEVER, WE MAKE NO WARRANTY OF MERCHANTABILITY OR ANY OTHER WARRANTY, EXPRESS OR IMPLIED, WITH RESPECT TO SUCH INFORMATION, AND WE ASSUME NO LIABILITY RESULTING FROM ITS USE. USERS SHOULD MAKE THEIR OWN INVESTIGATIONS TO DETERMINE THE SUITABILITY OF THE INFORMATION FOR THEIR PARTICULAR PURPOSES. IN NO EVENT SHALL SAMCHEM PRASANDHA BE LIABLE FOR ANY CLAIMS, LOSSES, OR DAMAGES OF ANY THIRD PARTY OR LOST PROFITS OR ANY SPECIAL, INDIRECT, INCIDENTAL, CONSEQUENTIAL OR EXEMPLARY DAMAGES, HOWSOEVER ARISING, EVEN IF SAMCHEM PRASANDHA HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

PRODUCT INFORMATION



Synonyms:

- Anon
- Anone
- ciclohexanona
- Cyclohexanon
- Cyclohexanone
- Cyclohexyl ketone
- Hexanon
- Hytrol O
- KETOHEXAMETHYLENE
- Nadone
- NSC 5711
- PIMELIC KETONE
- Pimelin ketone
- Sextone
- UN 1915
- UN 1915

www.samchemprasandha.com

Cyclohexanone is the organic compound with the formula $(CH_2)_5CO$. The molecule consists of six-carbon cyclic molecule with a <u>ketone</u> functional group. This colorless oil has an odor reminiscent of peardrop sweets as well as acetone. Over time, samples assume a yellow color due to oxidation. Cyclohexanone is slightly soluble in water (5-10 g/100 mL), but miscible with common organic solvents. Billions of kilograms are produced annually, mainly as a precursor to nylon.

Production

Cyclohexanone is produced by the oxidation of cyclohexane in air, typically using cobalt catalysts:^[4]

$$C_6H_{12} + O_2 \rightarrow (CH_2)_5CO + H_2O$$

This process co-forms cyclohexanol, and this mixture, called "KA oil" for ketone-alcohol oil, is the main feedstock for the production of adipic acid. The oxidation involves radicals and the intermediacy of the hydroperoxide $C_6H_{11}O_2H$. In some cases, purified cyclohexanol, obtained by hydration of cyclohexene, is the precursor. Alternatively, cyclohexanone can be produced by the partial hydrogenation of phenol:

$$C_6H_5OH + 2 H_2 \rightarrow (CH_2)_5CO$$

This process can also be adjusted to favor the formation of cyclohexanol.

Laboratory methods

Cyclohexanone can be prepared from cyclohexanol by oxidation with chromic oxide.

| Typical Properties | |
|--|-----------|
| Property | Value |
| Boiling point | 156°C |
| Melting point | -32.1°C |
| Relative density (water = 1) | 0.95 |
| Solubility in water, g/100 ml at 20°C | 8.7 |
| Vapour pressure, Pa at 20°C | 500 |
| Relative vapour density (air = 1) | 3.4 |
| Relative density of the vapour/air-mixture at 20°C (air = 1) | 1.01 |
| Flash point | 44°C c.c. |
| Auto-ignition temperature | 420°C |
| Explosive limits, vol% in air : 1.1 (at 100°C) | -9.4 |

Stability and Reactivity

Stability: Stable under ordinary conditions of use and storage.

Hazardous Decomposition Products: Carbon dioxide and carbon monoxide may form when heated to

decomposition.

Hazardous Polymerization: Will not occur.

Incompatibilities: Strong oxidizing agents. May cause spontaneous ignition and violent reaction. May attack

plastics, resins, and rubber.

Conditions to Avoid: Heat, flames, ignition sources and incompatibles.

Fax : 62-21-55952994

Hazards Identification

Emergency Overview

WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. AFFECTS CENTRAL NERVOUS SYSTEM, LIVER AND KIDNEYS. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT.

Health Rating: 2 - Moderate (Life) Flammability Rating: 2 - Moderate Reactivity Rating: 1 - Slight Contact Rating: 3 - Severe (Life)

Lab Protective Equip: GOGGLES & SHIELD; LAB COAT & APRON; VENT HOOD; PROPER GLOVES; CLASS B

EXTINGUISHER

Storage Color Code: Red (Flammable)

Potential Health Effects

Inhalation:

Causes irritation to the respiratory tract. Symptoms may include coughing, shortness of breath. High concentrations have a narcotic effect. Irritation effects normally prevent exposures high enough to cause systemic effects.

Ingestion:

May produce abdominal pain, nausea. Aspiration into lungs can produce severe lung damage and is a medical emergency. Other symptoms expected to parallel inhalation.

Skin Contact:

Causes irritation to skin. Symptoms include redness, itching, and pain. May be absorbed through the skin with possible systemic effects.

Eye Contact:

Vapors may cause irritation. Contact may cause corneal injury.

Chronic Exposure:

Prolonged or repeated exposure may cause skin rash or dermatitis. Damage to the liver and kidneys may occur.

Aggravation of Pre-existing Conditions:

Persons with pre-existing skin, eye or central nervous system disorders, or impaired liver, kidney, or pulmonary function may be more susceptible to the effects of this substance.

First Aid Measures

Inhalation:

Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Call a physician.

Ingestion:

Give large amounts of water to drink. Never give anything by mouth to an unconscious person. Get medical attention.

Skin Contact:

In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Call a physician.

Eye Contact:

Immediately flush eyes with plenty of water for at least 15 minutes, lifting lower and upper eyelids occasionally. Get medical attention immediately.

Fax: 62-21-55952994

Note to Physician:

In small ingestions the major concern is aspiration and gastrointestinal decontamination is not recommended. With larger ingestions there is potential for systemic toxicity from gastrointestinal absorption and decontamination is suggested, keeping in mind that aspiration is still a concern.

Fire Fighting Measures

Fire:

Flash point: 43.9°C (111°F)

Autoignition temperature: 420°C (788°F) Flammable limits in air % by volume:

lel: 1.1; uel: 9.4

Flammable. (lel @ 100°C)

Explosion:

Above flash point, vapor-air mixtures are explosive within flammable limits noted above. Vapors can flow along surfaces to distant ignition source and flash back. Contact with strong oxidizers may cause fire. Sealed containers may rupture when heated. Sensitive to static discharge.

Fire Extinguishing Media:

Dry chemical, foam or carbon dioxide. Water spray may be used to keep fire exposed containers cool, dilute spills to nonflammable mixtures, protect personnel attempting to stop leak and disperse vapors.

Special Information:

In the event of a fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus with full facepiece operated in the pressure demand or other positive pressure mode.

Accidental Release Measures

Ventilate area of leak or spill. Remove all sources of ignition. Wear appropriate personal protective equipment as specified in Section 8. Isolate hazard area. Keep unnecessary and unprotected personnel from entering. Contain and recover liquid when possible. Use non-sparking tools and equipment. Collect liquid in an appropriate container or absorb with an inert material (e. g., vermiculite, dry sand, earth), and place in a chemical waste container. Do not use combustible materials, such as saw dust. Do not flush to sewer! If a leak or spill has not ignited, use water spray to disperse the vapors, to protect personnel attempting to stop leak, and to flush spills away from exposures. US Regulations (CERCLA) require reporting spills and releases to soil, water and air in excess of reportable quantities. The toll free number for the US Coast Guard National Response Center is (800) 424-8802.

Handling and Storage

Protect against physical damage. Store in a cool, dry well-ventilated location, away from any area where the fire hazard may be acute. Outside or detached storage is preferred. Separate from incompatibles. Containers should be bonded and grounded for transfers to avoid static sparks. Storage and use areas should be No Smoking areas. Use non-sparking type tools and equipment, including explosion proof ventilation. Containers of this material may be hazardous when empty since they retain product residues (vapors, liquid); observe all warnings and precautions listed for the product.

Phone : 62-21-55952991 (hunting)
Fax : 62-21-55952994

Exposure Controls/Personal Protection

Airborne Exposure Limits:

-OSHA Permissible Exposure Limit (PEL): 50 ppm

-ACGIH Threshold Limit Value (TLV): 20 ppm (TWA) 50 ppm (STEL), skin, A3 - Confirmed animal carcinogen with unknown relevance to humans

Ventilation System:

A system of local and/or general exhaust is recommended to keep employee exposures below the Airborne Exposure Limits. Local exhaust ventilation is generally preferred because it can control the emissions of the contaminant at its source, preventing dispersion of it into the general work area. Please refer to the ACGIH document, *Industrial Ventilation*, *A Manual of Recommended Practices*, most recent edition, for details.

Personal Respirators (NIOSH Approved):

If the exposure limit is exceeded and engineering controls are not feasible, a half-face organic vapor respirator may be worn for up to ten times the exposure limit, or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. A full-face piece organic vapor respirator may be worn up to 50 times the exposure limit, or the maximum use concentration specified by the appropriate regulatory agency or respirator supplier, whichever is lowest. For emergencies or instances where the exposure levels are not known, use a full-face piece positive-pressure, air-supplied respirator. WARNING: Air-purifying respirators do not protect workers in oxygen-deficient atmospheres.

Skin Protection:

Wear impervious protective clothing, including boots, gloves, lab coat, apron or coveralls, as appropriate, to prevent skin contact.

Eye Protection:

Use chemical safety goggles and/or a full face shield where splashing is possible. Maintain eye wash fountain and quick-drench facilities in work area.

Other Information

NFPA Ratings: Health: 1 Flammability: 2 Reactivity: 0

Label Hazard Warning:

WARNING! FLAMMABLE LIQUID AND VAPOR. HARMFUL IF SWALLOWED, INHALED OR ABSORBED THROUGH SKIN. AFFECTS CENTRAL NERVOUS SYSTEM, LIVER AND KIDNEYS. CAUSES IRRITATION TO SKIN, EYES AND RESPIRATORY TRACT

Label Precautions:

Avoid contact with eyes, skin and clothing.

Avoid breathing vapor or mist.

Keep container closed.

Keep away from heat, sparks and flame.

Wash thoroughly after handling.

Use only with adequate ventilation.

Label First Aid:

If swallowed, give large amounts of water to drink. Never give anything by mouth to an unconscious person. If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. In case of contact, immediately flush eyes or skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. In all cases call a physician.

Fax: 62-21-55952994