



Safety Data Sheet

Cyclohexanone-3,3,4,4,5,5-d₆

Section 1. Chemical product and company identifications

Product code: D-6107

Chemical formula: C₆H₄D₆O

CAS: 54513-99-4

CAS (unlabelled): 108-94-1

Synonyms: Ketoexamethylene

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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Phone: 514-697-6254

Toll-Free (Canada & USA): 1-800-565-4696

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Website: www.cdnisotopes.com

In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid

Warning: Flammable liquid and vapour. Harmful if swallowed, in contact with skin or inhaled. Causes skin irritation. Causes serious eye damage.

Routes of entry: Inhalation, ingestion, skin and eyes

GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

GHS Classification:

- Flammable liquids (Category 3)
- Acute toxicity, Oral (Category 4)
- Acute toxicity, Inhalation (Category 4)
- Acute toxicity, Dermal (Category 4)
- Skin irritation (Category 2)
- Serious eye damage (Category 1)

GHS Label elements:

- Pictograms:   
- Signal word: Danger

Hazards statement:

- H226 Flammable liquid and vapour.
- H302 + H312 + H332 Harmful if swallowed, in contact with skin or inhaled.
- H315 Causes skin irritation.
- H318 Causes serious eye damage.

Precautionary statement:

- P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P302 + P350 IF ON SKIN: Wash with plenty of soap and water.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- P317 Get medical help.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
Cyclohexanone-3,3,4,4,5,5-d ₆	54513-99-4	> 98

Section 4. First aid measures

Eye contact: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

Skin contact: Wash off with soap and plenty of water. Consult a physician.

Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

Ingestion: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Section 5. Firefighting measures

Flammability of the product: Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

Lower explosion limit: 1.1 Vol%

Upper explosion limit: 9.4 Vol%

Auto-ignition temperature: 420 °C (788 °F)

Flash point: 44 °C (111 °F)

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.

Firefighting media and instructions: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Section 6. Accidental release measures

Personal precautions: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

Environmental precautions: Do not let product enter drains.

Methods for cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking.

Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources. Protect from light.

Section 8. Exposure Controls, Personal Protections

Engineering controls: Use mechanical exhaust or laboratory fumehood to avoid exposure.

Eyes: Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).

Respiratory: Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).

Hands: Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Skin/body: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Section 9. Physical and chemical properties (unlabelled)

Molecular weight: 98.14 g/mol

Physical status: Liquid

Color: Colorless

Odour: Mint-like

Density: 0.947 g/cm³

Melting point: -47 °C (-53 °F)

Boiling point: 155 °C (311 °F)

Vapour pressure: 4.5 hPa (3.4 mmHg) at 20 °C (68 °F)

Vapour density: 3.4 (Air = 1)

Partition coefficient (octanol/water): log Pow: 0.81

Water solubility: 86 g/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing agents.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.

Reactivity conditions: Heat, flames and sparks.

Section 11. Toxicological information (unlabelled)

Toxicological data: Cyclohexanone

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
Cyclohexanone	108-94-1	Oral - Rat - 1,534 mg/kg Dermal - Rabbit - 947 mg/kg	Inhalation - Rat - 4 h - 8,000 ppm

Potential acute effects

- **Eyes:** Causes serious eye damage.
- **Skin:** Harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** Harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Harmful if swallowed.

Potential chronic effects

- **Carcinogenic effects:** This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification. IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Cyclohexanone). ACGIH: A3 - Animal carcinogen.
- **Mutagenic effects:** Genotoxicity in vitro - Ames test - S. typhimurium - with and without metabolic activation - negative.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
Cyclohexanone	820 mg/l EC50	Daphnia magna	24 h

Effects on environment: No data available.

Mobility: No data available.

Environmental precautions: No data available.

Persistence and degradability: Aerobic. Result: 90 - 100 % - Readily biodegradable. Method: OECD Test guideline 301F.

Bioaccumulative potential: No data available.

Section 13. Disposal considerations

Waste disposal: Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Cyclohexanone

UN number: UN1915

Class: 3

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 2
Flammable: 2
Reactivity: 0
Special conditions: None

Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous

U.S. Federal regulations:

TSCA 8(b) inventory: Cyclohexanone

SARA 302/304/311/312 extremely hazardous substances: Not Listed

SARA 302/304 emergency planning and notification: Not Listed

SARA 302/304/311/312 hazardous chemicals: Not Listed

SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Listed

CWA (Clean Water Act) 307: Not Listed

CWA (Clean Water Act) 311: Not Listed

CAA (Clean Air Act) 112 accidental release prevention: Not Listed

CAA (Clean Air Act) 112 regulated flammable substances: Not Listed

CAA (Clean Air Act) 112 regulated toxic substances: Not Listed

State regulations:

DEA List I Chemicals (Precursor Chemicals): Not Listed

DEA List II Chemicals (Essential Chemicals): Not Listed

Substances in Massachusetts: Listed

Dangerous substances in New Jersey: Listed

New York – Dangerous substances with acute effects: Not Listed

Dangerous substances in Pennsylvania – right to know: Listed

WHMIS (Canada):



B3 - Combustible Liquid



D2B - Toxic material causing other toxic effects

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part 1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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Elaborated by: Toxyscan Inc., 1-866-780-0599

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