

Chemical Safety Data Sheet MSDS / SDS

Cyclohexanone-2,2,6,6-d4Revision Date:2026-09-12 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : Cyclohexanone-2,2,6,6-d4
CBnumber : CB4676959
CAS : 1006-03-7
Synonyms : CYCLOHEXANONE-2,2,6,6-D4

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P233 Keep container tightly closed.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ventilating/lighting/.../equipment.
P242 Use only non-sparking tools.

Hazard statements

H226 Flammable liquid and vapour
H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: Cyclohexanone-2,2,6,6-d4
Synonyms	: CYCLOHEXANONE-2,2,6,6-D4
CAS	: 1006-03-7
MF	: C6H6D4O
MW	: 102.17

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO2) Foam Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®).

Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['Cyclohexanone- 2,2,6,6-d4', '1006-03-7', 'PC-TWA', '50 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']	['', 'Remarks', 'Skin', None, None]
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Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis']	['Cyclohexanone- 2,2,6,6-d4', '1006-03-7', '1,2- Cyclohexan ediol', '80 mg/l', 'Urine', 'ACGIH - Biological Exposure Indices (BEI)']	['', 'Remarks', 'End of shift at end of workweek', None, None, None]	['', 'Cyclohexan ol', '8 mg/l', 'Urine', 'ACGIH - Biological Exposure Indices (BEI)']	['', 'End of shift (As soon as possible after exposure ceases)', None, None, None]
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8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 120 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	clear, liquid
b) Color	colorless
c) Odor	No data available
d) Melting point/freezing point	Melting point/range: -47 °C - lit.
e) Initial boiling point and boiling range	153 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	44 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	0.986 g/mL at 25 °C 0.986 g/cm ³ at 25 °C
Relative density	0.986 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none
Appearance	Colorless to light yellow Liquid

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Stable

10.2 Possibility of hazardous reactions

Risk of explosion with:

Nitric acid hydrogen peroxide

Oxidizing agents mineral acids

10.3 Conditions to avoid

Heating.

10.4 Incompatible materials

No data available

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 1,620 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: Cyclohexanone

Symptoms: Stomach/intestinal disorders, Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

LC50 Inhalation - Rat - male and female - 4 h - > 6.2 mg/l - vapor

Remarks: (ECHA)

The value is given in analogy to the following substances: Cyclohexanone

Symptoms: In high doses:, Irritation symptoms in the respiratory tract.

LD50 Dermal - Rabbit - 1,100 mg/kg

Remarks: (External MSDS)

The value is given in analogy to the following substances: Cyclohexanone

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h (OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: Cyclohexanone

Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - In vitro study

Result: Irreversible effects on the eye

Remarks: (ECHA)

The value is given in analogy to the following substances: Cyclohexanone

Remarks: Risk of corneal clouding.

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: Cyclohexanone

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: CyclohexanoneTest

Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: CyclohexanoneTest

Type: unscheduled DNA synthesis assay

Test system: human diploid fibroblasts

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 482

Result: negative

Remarks: The value is given in analogy to the following substances: Cyclohexanone

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: Cyclohexanone

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory Tract

Remarks: The value is given in analogy to the following substances: Cyclohexanone

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 3 Months - NOAEL (No observed adverse effect level) - 143 mg/kg

Remarks: The value is given in analogy to the following substances: Cyclohexanone

Prolonged or repeated exposure to skin causes defatting and dermatitis., burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting,

Central nervous system depression, Incoordination., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

After absorption of large quantities:

Headache

Salivation

Nausea

Vomiting

Dizziness narcosis

Coma

The following applies to ketones in general: when vapours/aerosols occur, mucosal irritations, coughing, and dyspnoea after inhalation. The absorption of large quantities leads to: CNS depression (narcosis). Repeated skin contact leads to a degreasing effect, with secondary inflammation possible. Toxic effects on the liver and kidneys cannot be excluded after high doses. The inhalation of droplets may result in the formation of oedemas in the respiratory tract.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 527 - 732 mg/l - 96 h (OECD Test Guideline 203)

Remarks: The value is given in analogy to the following substances:

Cyclohexanone

Toxicity to bacteria Remarks: The value is given in analogy to the following substances:

Cyclohexanone (Cyclohexanone-2,2,6,6-d4)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 90 - 100 % - Readily biodegradable.

(OECD Test Guideline 301F)

Remarks: The value is given in analogy to the following substances:

Cyclohexanone

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1915

IMDG: 1915

IATA-DGR: 1915

14.2 UN proper shipping name

ADR/RID: CYCLOHEXANONE

IMDG: CYCLOHEXANONE

IATA-DGR: Cyclohexanone

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA-DGR: III

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.