SAFETY DATA SHEET

Version 6.6
Revision Date 09/09/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Cyclohexanone-2,2,6,6-d_4

Product Number : 176613
Brand : Aldrich
CAS-No. : 1006-03-7

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312

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Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word Danger

Hazard Statements

H226	Flammable liquid and vapor.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.

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.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : $C_6D_4H_6O$
Molecular weight : 102.13 g/mol
CAS-No. : 1006-03-7
EC-No. : 686-038-4

Component	Classification	Concentration
Cyclohexanone-2,2,6,6-d4		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H302, H332, H312, H315, H318, H335	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

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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.

5.4 Further information

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

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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

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		STEL	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	25 ppm 100 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	50 ppm 200 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	25 ppm 100 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

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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-Cyclohexanediol	80 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			
		Cyclohexanol	8 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

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 EN 16523-1 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 EN 16523-1 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.

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Respiratory protection
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds
The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.
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

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: clear, liquid Color: colorless
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/ range: -47 °C (-53 °F) - lit.
f)	Initial boiling point and boiling range	153 °C 307 °F - lit.
g)	Flash point	44 °C (111 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	0.986 g/mL at 25 °C (77 °F)0.986 g/cm3 at 25 °C (77 °F)
	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	No data available
q)	Decomposition	No data available

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temperature

r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature) .
Stable

10.3 Possibility of hazardous reactions

Risk of explosion with:
Nitric acid
hydrogen peroxide
Oxidizing agents
mineral acids

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
No data available

10.6 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.

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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

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is

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identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

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
No data available

Aspiration hazard
No data available

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.

Stomach - Irregularities - Based on Human Evidence

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Stomach - Irregularities - Based on Human Evidence

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

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SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 1915 Class: 3 Packing group: III
Proper shipping name: Cyclohexanone
Reportable Quantity (RQ): 5000 lbs
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 1915 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: CYCLOHEXANONE

IATA
UN number: 1915 Class: 3 Packing group: III
Proper shipping name: Cyclohexanone

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Cyclohexanone-2,2,6,6-d4	1006-03-7	5000	5000
Cyclohexanone-2,2,6,6-d4	1006-03-7	100	100 (F003)

SARA 304 Extremely Hazardous Substances Reportable Quantity
This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity
This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard
Chronic Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

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US State Regulations

Massachusetts Right To Know

Cyclohexanone-2,2,6,6-d4	1006-03-7

Pennsylvania Right To Know

Cyclohexanone-2,2,6,6-d4	1006-03-7

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Details in analogy to the undeuterated compound.

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