

SAFETY DATA SHEET

Version 6.8
Revision Date 09/06/2024
Print Date 09/07/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Cyclohexane-d₁₂
Product Number : 151866
Brand : Aldrich
Index-No. : 601-017-00-1
CAS-No. : 1735-17-7

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 2), H225
Skin irritation (Category 2), H315
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

Aldrich - 151866

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Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

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

| | |
|------|---|
| H225 | Highly flammable liquid and vapor. |
| H304 | May be fatal if swallowed and enters airways. |
| H315 | Causes skin irritation. |
| H336 | May cause drowsiness or dizziness. |
| H410 | Very toxic to aquatic life with long lasting effects. |

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. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P273 | Avoid release to the environment. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P310 | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. |
| 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. |
| P331 | Do NOT induce vomiting. |
| 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. |
| P391 | Collect spillage. |
| 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

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₆D₁₂
Molecular weight : 96.23 g/mol
CAS-No. : 1735-17-7
EC-No. : 217-077-3
Index-No. : 601-017-00-1

| Component | Classification | Concentration |
|-----------------------------------|---|---------------|
| cyclohexane-d₁₂ | | |
| | Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 M-Factor - Aquatic Acute: 1 | <= 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. Call in physician.

In case of skin contact

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

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) 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.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

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 carefully 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.

hygroscopic

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 |
|-----------------------------|-----------|-------|------------------------------------|---|
| cyclohexane-d ₁₂ | 1735-17-7 | TWA | 100 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | TWA | 300 ppm 1,050 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | TWA | 300 ppm 1,050 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | PEL | 300 ppm 1,050 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

Biological occupational exposure limits

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|-----------------------------|-----------|---------------------------------|-------------------|---------------------|---|
| cyclohexane-d ₁₂ | 1735-17-7 | 1,2-Cyclohexanediol | 50mg/g creatinine | Urine | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | End of shift at end of workweek | | | |

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). Safety glasses

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: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

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: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 30 min

Material tested: KCL 741 Dermatril® L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur 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: 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: 6.5 °C (43.7 °F) |
| f) Initial boiling point and boiling range | 80.7 °C 177.3 °F - lit. |
| g) Flash point | -18 °C (-0.40 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 9 %(V) Lower explosion limit: 1 %(V) |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Density | 0.893 g/mL at 25 °C (77 °F) - lit.0.893 g/cm ³ at 25 °C (77 °F) - lit. |
| 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 temperature | No data available |
| 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

Vapors may form explosive mixture with air.

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:
nitrogen dioxide

Risk of ignition or formation of inflammable gases or vapours with:
Strong oxidizing agents

10.4 Conditions to avoid

Warming.

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 and female - > 5,000 mg/kg
(OECD Test Guideline 401)

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

Symptoms: gastric pain, Stomach/intestinal disorders

LC50 Inhalation - Rat - male and female - 4 h - 19.07 mg/l - vapor

(OECD Test Guideline 403)

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

Symptoms: Possible damages:, Irritation symptoms in the respiratory tract., Inhalation may lead to the formation of oedemas in the respiratory tract.

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

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

Skin corrosion/irritation

Remarks: Causes skin irritation.

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

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

Germ cell mutagenicity

Test Type: Ames test

Test system: 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: Cyclohexane

In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

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: Cyclohexane

Test Type: Chromosome aberration test

Species: Rat

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: OECD Test Guideline 475

Result: negative

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

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is 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 drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

Central nervous system depression, Drowsiness, Irritability, Dizziness, Gastrointestinal disturbance, Lung irritation, chest pain, pulmonary edema, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After uptake of large quantities:

Unconsciousness

Damage to:

Lungs

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - 4.53 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: Cyclohexane |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 0.9 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: Cyclohexane |
| Toxicity to algae | ErC50 - Pseudokirchneriella subcapitata (green algae) - > 4.425 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: Cyclohexane |

12.2 Persistence and degradability

| | |
|------------------|---|
| Biodegradability | aerobic - Exposure time 28 d Result: 77 % - Readily biodegradable. (OECD Test Guideline 301F) Remarks: The value is given in analogy to the following substances: Cyclohexane |
|------------------|---|

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

Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

Change in the flavour characteristics of fish protein.

Discharge into the environment must be avoided.

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: 1145 Class: 3 Packing group: II
Proper shipping name: Cyclohexane
Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1145 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: CYCLOHEXANE
Marine pollutant : yes

IATA

UN number: 1145 Class: 3 Packing group: II
Proper shipping name: Cyclohexane

SECTION 15: Regulatory information

CERCLA Reportable Quantity

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| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|-----------------------------|-----------|--------------------|-----------------------------|
| cyclohexane-d ₁₂ | 1735-17-7 | 1000 | 1000 |

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 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

| | | |
|-----------------------------|-----------|------------------|
| cyclohexane-d ₁₂ | 1735-17-7 | >= 90 - <= 100 % |
|-----------------------------|-----------|------------------|

US State Regulations

Massachusetts Right To Know

| | |
|-----------------------------|-----------|
| cyclohexane-d ₁₂ | 1735-17-7 |
|-----------------------------|-----------|

Pennsylvania Right To Know

| | |
|-----------------------------|-----------|
| cyclohexane-d ₁₂ | 1735-17-7 |
|-----------------------------|-----------|

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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