

SAFETY DATA SHEET

Version 6.12
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 1,4-Cyclohexadiene

Product Number : 125415
Brand : Aldrich
CAS-No. : 628-41-1

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
Germ cell mutagenicity (Category 1B), H340
Carcinogenicity (Category 1A), H350
Specific target organ toxicity - repeated exposure (Category 1), Blood, H372

Short-term (acute) aquatic hazard (Category 3), H402

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.
H340	May cause genetic defects.
H350	May cause cancer.
H372	Causes damage to organs (Blood) through prolonged or repeated exposure.
H402	Harmful to aquatic life.

Precautionary Statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
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.
P260	Do not breathe mist or vapors.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
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

Synonyms : 1,4-Dihydrobenzene

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Formula : C₆H₆
 Molecular weight : 80.13 g/mol
 CAS-No. : 628-41-1
 EC-No. : 211-043-1

Component	Classification	Concentration
benzene		
	Flam. Liq. 2; Skin Irrit. 2; Eye Irrit. 2A; Muta. 1B; Carc. 1A; STOT RE 1; Asp. Tox. 1; Aquatic Chronic 3; H225, H315, H319, H340, H350, H372, H304, H412	>= 1 - < 5 %

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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. 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

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. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability Recommended storage temperature

2 - 8 °C

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
benzene	71-43-2	TWA	0.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Leukemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed human carcinogen Danger of cutaneous absorption		
		STEL	2.5 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Leukemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed human carcinogen Danger of cutaneous absorption		
		TWA	10 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.40-1969		
		CEIL	25 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.40-1969		
		Peak	50 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.40-1969		
		See 1910.1028. See Table Z-2 for the limits applicable in the operations or sectors excluded in 1910.1028 The final benzene standard in 1910.1028 applies to all occupational exposures to benzene except some subsegments of industry where exposures are consistently under the action level (i.e., distribution and sale of fuels,		

		sealed containers and pipelines, coke production, oil and gas drilling and production, natural gas processing, and the percentage exclusion for liquid mixtures); for the excepted subsegments, the benzene limits in Table Z-2 apply.		
		TWA	0.1 ppm	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen See Appendix A		
		ST	1 ppm	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen See Appendix A		

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

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

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: 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	No data available
f) Initial boiling point and boiling range	88 - 89 °C 190 - 192 °F - lit.
g) Flash point	-7 °C (19 °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	0.847 g/mL 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	No data available

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) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

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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

Acute toxicity estimate Oral - > 5,000 mg/kg

(Calculation method)

Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: 1 - Group 1: Carcinogenic to humans (benzene)

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

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available (Cyclohexa-1,4-diene)

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Cyclohexa-1,4-diene)

Stomach - Irregularities - Based on Human Evidence

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SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available (Cyclohexa-1,4-diene)

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

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: 3295 Class: 3 Packing group: II

Proper shipping name: Hydrocarbons, liquid, n.o.s.

Reportable Quantity (RQ): 333 lbs

Reportable Quantity (RQ): 10 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 3295

Class: 3

Packing group: II EMS-No: F-

E, S-D

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Proper shipping name: HYDROCARBONS, LIQUID, N.O.S.

IATA

UN number: 3295 Class: 3 Packing group: II
Proper shipping name: Hydrocarbons, liquid, n.o.s.

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
benzene	71-43-2	10	333
benzene	71-43-2	10	10 (D018)

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
Acute Health Hazard
Chronic Health Hazard

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

benzene 71-43-2 >= 1 - < 5 %

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

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 : All substances listed as active on the 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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