SAFETY DATA SHEET

Version 6.7
Revision Date 08/08/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 1,3-Cyclohexanedione

Product Number : C101605
Brand : Aldrich
CAS-No. : 504-02-9

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute toxicity (Oral) : Category 4

Serious eye damage : Category 1

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Short-term (acute) aquatic hazard : Category 3

Long-term (chronic) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :

Signal Word : Danger

Hazard Statements : H302 Harmful if swallowed.
H318 Causes serious eye damage.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements :

Prevention:

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 eye protection/ face protection.

Response:

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Cyclohexane-1,3-dione	504-02-9*	>= 90 - <= 100	-

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* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice	:	Show this 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.
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.
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
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	:	Water Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	:	Carbon oxides

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Hydrogen chloride gas

Sodium oxides

Specific extinguishing methods	:	No data available
Further information	:	Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains.
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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions	:	Tightly closed. Dry.
Storage class	:	13, Non Combustible Solids
Recommended storage	:	36 - 46 °F / 2 - 8 °C

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temperature

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts 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.

Recommended Filter type: : Filter type P2

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.

Hand protection

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Full contact
Manufacturer	:	KCL 741 Dermatril® L

Material	:	Nitrile rubber
Break through time	:	480 min
Glove thickness	:	0.11 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.
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).

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Eye 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 and body protection	:	protective clothing
Hygiene measures	:	Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	powder, finecrystalline
Color	:	beige
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	214 - 221 °F / 101 - 105 °C Method: lit.
Boiling point/boiling range	:	No data available
Flash point	:	No data available
Evaporation rate	:	No data available
Flammability (solid, gas)	:	The product is not flammable. Method: Flammability (solids) GLP: yes
Burning rate	:	No data available
Self-ignition	:	> 266 °F / > 130 °C Method: Relative self-ignition temperature for solids GLP: yes
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapor pressure	:	No data available

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Relative vapour density	:	No data available
Relative density	:	ca. 1.27 (68 °F / 20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.3 GLP: yes
Density	:	1.08 g/cm3 (196 °F / 91 °C)
Solubility(ies) Water solubility	:	100 g/l completely soluble (68 °F / 20 °C) Method: Regulation (EC) No. 440/2008, Annex, A.6 GLP: yes
Partition coefficient: n-octanol/water	:	log Pow: ca. 0.461 (ca. 70.5 °F / 21.4 °C) Method: OECD Test Guideline 107 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, dynamic	:	No data available
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Method: Explosive properties GLP: yes
Oxidizing properties	:	Method: Regulation (EC) No. 440/2008, Annex, A.17 GLP: yes none
Surface tension	:	ca. 69.9 mN/m, 1.01 g/l, 72 °F / 22 °C, Surface tension, GLP: yes
Molecular weight	:	112.13 g/mol
Particle characteristics Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	The following applies in general to flammable organic substances and mixtures: in correspondingly fine

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		distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Contains the following stabiliser(s):	:	sodium chloride (>1 - <3 %)
Possibility of hazardous reactions	:	No data available
Conditions to avoid	:	no information available
Incompatible materials	:	Strong oxidizing agents
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 - 1,600 - 2,500 mg/kg
Remarks: (ECHA)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Mild skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Severe irritations - 10 s
Remarks: (ECHA)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

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

Carcinogenicity

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

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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
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Cyclohexane-1,3-dione:

Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 24 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	:	ErC50 (Desmodesmus subspicatus (green algae)): 35 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes NOEC (Desmodesmus subspicatus (green algae)): 12.5 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes

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Persistence and degradability

Components:

Cyclohexane-1,3-dione:

Biodegradability	:	aerobic Concentration: 1.5 mg/l Result: Not inherently biodegradable. Biodegradation: 28 % Exposure time: 28 d Method: OECD Test Guideline 301D GLP: yes

Bioaccumulative potential

Components:

Cyclohexane-1,3-dione:

Partition coefficient: n-octanol/water	:	log Pow: ca. 0.461 (ca. 70.5 °F / 21.4 °C) pH: 3.2 Method: OECD Test Guideline 107 GLP: yes Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	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

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

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49 CFR Road
Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

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 : No SARA Hazards

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.

US State Regulations

Massachusetts Right To Know

sodium chloride	7647-14-5

Maine Chemicals of High Concern

sodium chloride	7647-14-5

Vermont Chemicals of High Concern

sodium chloride	7647-14-5

Washington Chemicals of High Concern

sodium chloride	7647-14-5

The components 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.

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SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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