

## SAFETY DATA SHEET

Version 6.3  
Revision Date 02/25/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****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

**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)**

Acute toxicity, Oral (Category 4), H302

Serious eye damage (Category 1), H318

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

Long-term (chronic) aquatic hazard (Category 3), H412

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 statement(s)	
H302	Harmful if swallowed.
H318	Causes serious eye damage.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
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.
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.
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 : Dihydroresorcinol

Formula : C<sub>6</sub>H<sub>8</sub>O<sub>2</sub>

Molecular weight : 112.13 g/mol

CAS-No. : 504-02-9

EC-No. : 207-980-0

Component	Classification	Concentration
<b>Cyclohexane-1,3-dione</b>		
	Acute Tox. 4; Eye Dam. 1; Aquatic Acute 3; Aquatic Chronic 3; H302, H318, H402, H412	<= 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

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

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Hydrogen chloride gas

Sodium oxides

Combustible.

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

**6.3 Methods and materials for containment and cleaning up**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

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**SECTION 7: Handling and storage****7.1 Precautions for safe handling****Advice on safe handling**

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Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

**Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

**Advice on protection against fire and explosion**

Provide appropriate exhaust ventilation at places where dust is formed.

**Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

**Storage stability**

Recommended storage temperature

2 - 8 °C

Storage class (TRGS 510): 13: Non Combustible Solids

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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**SECTION 8: Exposure controls/personal protection**

**8.1 Control parameters**

**Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

**8.2 Exposure controls**

**Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

**Personal protective equipment**

**Eye/face protection**

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

**Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Body Protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as

a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### **Control of environmental exposure**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: powder, finecrystalline Color: beige
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 101 - 105 °C (214 - 221 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	The product is not flammable. - Flammability (solids)
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Relative density	ca.1.27 at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.3
n) Water solubility	100 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6 - completely soluble
o) Partition coefficient: n-octanol/water	log Pow: ca.0.461 at ca.21.4 °C (ca.70.5 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	> 130 °C (> 266 °F) - Relative self-ignition temperature for solids
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**

Surface tension ca.69.9 mN/m at 1.01g/l at 22 °C (72 °F) - Surface tension

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

Contains the following stabilizer(s):

sodium chloride (>1 - <3 %)

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## 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

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

Ames test

Salmonella typhimurium

Result: negative

#### Carcinogenicity

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- 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**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

Not available

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

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**SECTION 12: Ecological information**

**12.1 Toxicity**

No data available

Toxicity to daphnia and other aquatic invertebrates      static test EC50 - Daphnia magna (Water flea) - 24 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae      static test ErC50 - Desmodesmus subspicatus (green algae) - 35 mg/l - 72 h (OECD Test Guideline 201)  
static test NOEC - Desmodesmus subspicatus (green algae) - 12.5 mg/l - 72 h (OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: 28 % - Not inherently biodegradable.  
(OECD Test Guideline 301D)

**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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life with long lasting effects.

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

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

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

#### Further information

Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

#### SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

#### SARA 313 Components

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.

#### SARA 311/312 Hazards

No SARA Hazards

#### Massachusetts Right To Know Components

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

#### Pennsylvania Right To Know Components

Cyclohexane-1,3-dione

CAS-No.  
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## SECTION 16: Other information

### Further information

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