

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Date of issue: 05.12.2016

Version 1.0

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No.	820367
Product name	1,3-Cyclohexanedione for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	504-02-9

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number	Please contact the regional company representation in your country.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Chronic aquatic toxicity, Category 3, H412

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

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Reduced labelling (≤125 ml)

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

CAS-No. 504-02-9

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	C ₆ H ₈ -1,3-(=O) ₂	C ₆ H ₈ O ₂ (Hill)
EC-No.	207-980-0	
Molar mass	112,12 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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Cyclohexane-1,3-dione (<= 100 %)		
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504-02-9	*)	
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Chronic aquatic toxicity, Category 3, H412

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3.2 Mixture

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Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

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

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

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed

We have no description of any toxic symptoms.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, 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

Combustible.

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

5.3 Advice for firefighters

Special protective equipment for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Recommended storage temperature see product label.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

Other protective equipment

protective clothing

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Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 1 (acc. to DIN 3181) for solid particles of inert substances

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.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	powder, finecrystalline
Colour	beige
Odour	No strong odour known.
Odour Threshold	No information available.
pH	No information available.
Melting point/range	101 - 105 °C
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.

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Vapour pressure	No information available.
Relative vapour density	No information available.
Density	No information available.
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	No information available.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

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strong oxidising agents

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

This information is not available.

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: Mild skin irritation

OECD Test Guideline 404

Eye irritation

This information is not available.

Sensitisation

Local lymph node assay (LLNA) Mouse

Result: negative

Method: OECD Test Guideline 429

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

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Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates

static test EC50 Daphnia magna (Water flea): 24 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

Toxicity to algae

static test EC50 Desmodesmus subspicatus (green algae): 35 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

static test NOEC Desmodesmus subspicatus (green algae): 12,5 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

No information available.

12.4 Mobility in soil

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No information 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

Additional ecological information

No ecological problems are to be expected when the product is handled and used with due care and attention.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard	SEVESO III
Legislation	Not applicable

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Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 10 - 13

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H412 Harmful to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

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Prevention

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Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.