

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 13.08.2018

Version 4.8

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

1.1 Product identifier

Catalogue No.	806913
Product name	DL-Mandelic acid for synthesis
REACH Registration Number	01-2120349224-60-XXXX
CAS-No.	90-64-2

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.**

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Serious eye damage, Category 1, H318

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 pictograms



Signal word

Danger

Hazard statements

H318 Causes serious eye damage.

Precautionary statements

Prevention

P260 Do not breathe dust.

P280 Wear eye protection.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H318 Causes serious eye damage.

Precautionary statements

P280 Wear eye protection.

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P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

CAS-No. 90-64-2

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	C ₆ H ₅ CH(OH)COOH	C ₈ H ₈ O ₃ (Hill)
EC-No.	210-277-1	
Molar mass	152,15 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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DL-2-hydroxy-2-phenylacetic acid (<= 100 %)

90-64-2	01-2120349224-60-XXXX	Serious eye damage, Category 1, H318
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For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

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. Immediately call in ophthalmologist.

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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

Irritation and corrosion
Risk of serious damage to eyes.
Cough, Gastrointestinal discomfort

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.

SECTION 6. Accidental release measures

6.1 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:

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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

Protected from light.

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.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

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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

Tightly fitting safety goggles

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.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

protective clothing

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Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful 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	crystals
Colour	white
Odour	weakly aromatic
Odour Threshold	No information available.
pH	2,3 at 10 g/l
Melting point/range	119 - 121 °C
Boiling point/boiling range	255 - 340 °C at 1.013 hPa Method: OECD Test Guideline 103 Decomposition
Flash point	No information available.

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Evaporation rate	No information available.
Flammability (solid, gas)	The product is not flammable. Flammability (solids)
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	0,01 Pa at 50 °C Method: OECD Test Guideline 104
Relative vapour density	No information available.
Density	1,31 g/cm ³ at 20,2 °C Method: OECD Test Guideline 109
Relative density	No information available.
Water solubility	139 g/l at 20 °C Method: OECD Test Guideline 105
Partition coefficient: n-octanol/water	log Pow: 0,5 (23 °C) OECD Test Guideline 107 Bioaccumulation is not expected.
Auto-ignition temperature	does not ignite
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.

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Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

Bulk density 750 kg/m³

Particle size Mean particle size
108,9 µm
Method: OECD Test Guideline 110

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

Sensitivity to light

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong reducing agents, strong alkalis, Acids, Alcohols, Amines, Ammonia, Acid anhydrides, Strong bases

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 5.000 mg/kg

OECD Test Guideline 401

The value is given in analogy to the following substances: (R)-(-)-mandelic acid

Symptoms: After swallowing: irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: No irritation

(External MSDS)

Eye irritation

Rabbit

Result: Causes serious eye damage.

OECD Test Guideline 405

The value is given in analogy to the following substances: (R)-(-)-mandelic acid

In vitro study

Result: Causes serious eye damage.

OECD Test Guideline 437

Causes serious eye damage.

Sensitisation

This information is not available.

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Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

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

EC50 Daphnia magna (Water flea): > 100 mg/l; 48 h

(External MSDS)

Toxicity to algae

Growth inhibition ErC50 Pseudokirchneriella subcapitata (green algae): > 100 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

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Growth inhibition NOEC *Pseudokirchneriella subcapitata* (green algae): > 100 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

Growth inhibition EC10 *Pseudokirchneriella subcapitata* (green algae): > 100 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

12.2 Persistence and degradability

Biodegradability

99 %; 28 d; aerobic

OECD Test Guideline 301F

Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,5 (23 °C)

OECD Test Guideline 107

Bioaccumulation is not expected.

12.4 Mobility in soil

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

Surface tension

69,8 mN/m

at 20 °C

Method: OECD Test Guideline 115

Additional ecological information

Discharge into the environment must be avoided.

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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

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

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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.

H318 Causes serious eye damage.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

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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.