

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 27.03.2013

Version 3.4

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

#### 1.1 Product identifier

Catalogue No.	806925
Product name	(S)-(+)-Mandelic acid for resolution of racemates 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.

#### 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 ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ).
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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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

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)

Serious eye damage, Category 1, H318

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

Classification (67/548/EEC or 1999/45/EC)

Xi                      Irritant    R41

For the full text of the R-phrases mentioned in this Section, see Section 16.

#### 2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H318 Causes serious eye damage.

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*Precautionary statements*

Prevention

P280 Wear eye protection.

P260 Do not breathe dust.

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.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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.

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. 17199-29-0

**Labelling (67/548/EEC or 1999/45/EC)**

Symbol(s)  Xi Irritant

R-phrase(s) 41 Risk of serious damage to eyes.

S-phrase(s) 22-26-39 Do not breathe dust. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection.

EC-No. 241-240-8

**Reduced labelling (≤125 ml)**

Symbol(s)  Xi Irritant

R-phrase(s) 41 Risk of serious damage to eyes.

S-phrase(s) 26-39 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection.

**2.3 Other hazards**

None known.

**SECTION 3. Composition/information on ingredients**

**3.1 Substance**

Formula	C <sub>6</sub> H <sub>5</sub> CH(OH)COOH	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> (Hill)
CAS-No.	17199-29-0	
EC-No.	241-240-8	
Molar mass	152,15 g/mol	

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

*Chemical Name (Concentration)*

CAS-No.                      Registration number                      Classification

(S)-(+)-mandelic acid (<= 100 % )

17199-29-0                      \*)

Serious eye damage, Category 1, H318

\*) 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.

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

**Hazardous components (1999/45/EC)**

*Chemical Name (Concentration)*

CAS-No.                      Classification

(S)-(+)-mandelic acid (<= 100 % )

17199-29-0                      Xi, Irritant; R41

For the full text of the R-phrases mentioned in this Section, see Section 16.

**3.2 Mixture**

not applicable

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**SECTION 4. First aid measures**

**4.1 Description of first aid measures**

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

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**

irritant effects, Risk of serious damage to eyes.

**4.3 Indication of any immediate medical attention and special treatment needed**

No information available.

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**SECTION 5. Firefighting measures**

**5.1 Extinguishing media**

*Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, 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.

Forms explosive mixtures with air on intense heating.

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.

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*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 substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. 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 empty into 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.

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**SECTION 7. Handling and storage**

**7.1 Precautions for safe handling**

*Advice on safe handling*

Observe label precautions.

*Hygiene measures*

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

**7.2 Conditions for safe storage, including any incompatibilities**

*Storage conditions*

Protected from light. Tightly closed. Dry.

Store at +15°C to +25°C.

**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.

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806925

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## 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](http://www.kcl.de)).

### *Other protective equipment*

protective clothing

### *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 empty into 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	2,1 at 60 g/l 20 °C

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Melting point	130 - 132 °C
Boiling point	No information available.
Flash point	> 190 °C
Evapouration rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: 0,57 (calculated) Bioaccumulation is not expected. (Lit.)
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	not applicable
Oxidizing properties	none

## 9.2 Other data

Bulk density	670 kg/m <sup>3</sup>
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## 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.

Forms explosive mixtures with air on intense heating.

### 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

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**10.4 Conditions to avoid**

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**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*

This information is not available.

*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: Eye irritation

(External MSDS)

Causes serious eye damage.

*Sensitisation*

This information is not available.

*Germ cell mutagenicity*

This information is not available.

*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.

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**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)

**12.2 Persistence and degradability**

*Biodegradability*

90 - 100 %; 14 d

(External MSDS)

Readily biodegradable.

**12.3 Bioaccumulative potential**

*Partition coefficient: n-octanol/water*

log Pow: 0,57

(calculated)

Bioaccumulation is not expected. (Lit.)

**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**

Discharge into the environment must be avoided.

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**SECTION 13. Disposal considerations**

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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**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

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**SECTION 15. Regulatory information**

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

*EU regulations*



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Major Accident Hazard Legislation	96/82/EC Directive 96/82/EC does not apply
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
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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
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Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals	not regulated
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Substances of very high concern (SVHC)	This product does not contain substances of very high concern above the respective regulatory limit (> 0.1 % (w/w) Regulation (EC) No 1907/2006 (REACH), Article 57).
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*National legislation*

Storage class	10 - 13
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## 15.2 Chemical Safety Assessment

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

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## SECTION 16. Other information

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

H318	Causes serious eye damage.
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### Full text of R-phrases referred to under sections 2 and 3

R41	Risk of serious damage to eyes.
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### Training advice

Provide adequate information, instruction and training for operators.

### 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](http://www.wikipedia.org).

### Regional representation

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

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*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.*