

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 05.11.2010

Version 3.5

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

1.1 Product identifier

Catalogue No.	806914
Product name	(R)-(-)-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 (www.merck-chemicals.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.

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; 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.

Precautionary statements

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

P260 Do not breathe dust.
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.

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.

CAS-No. 611-71-2

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. 210-276-6

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.

3. Composition/information on ingredients

Formula	C ₆ H ₅ CH(OH)COOH	C ₈ H ₈ O ₃ (Hill)
CAS-No.	611-71-2	
EC-No.	210-276-6	
Molar mass	152,15 g/mol	

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.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

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

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
irritant effects

4.3 Indication of immediate medical attention and special treatment needed
No information available.

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, Dry powder, Water

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 material

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 fire-fighters

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.

6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Ensure adequate ventilation.

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 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 7.2 and 10.5).

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.

7. Handling and storage

7.1 Precautions for safe handling

Observe label precautions.

7.2 Conditions for safe storage, including any incompatibilities

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

Protected from light. Tightly closed. Dry.

Store at +15°C to +25°C.

7.3 Specific end uses

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

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.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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

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

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

properly documented.

Environmental exposure controls

Do not empty into drains.

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
Melting point	130 - 132 °C
Boiling point	No information available.
Flash point	> 190 °C
Evaporation 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 Method: (calculated) Bioaccumulation is not expected (log Pow <1). (Lit.)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	No information available.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

Oxidizing properties No information available.

9.2 Other data

Bulk density 670 kg/m³

10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
The following applies in general to flammable organic substances and preparations: 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, alkalines, strong reducing agents

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 rat
Dose: 5.000 mg/kg
(External MSDS)

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Skin irritation

rabbit
Result: No irritation
(External MSDS)

Eye irritation

rabbit
Result: Eye irritation
(External MSDS)
Causes serious eye damage.

Genotoxicity in vitro

Ames test
Result: negative
(External MSDS)

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

11.2 Further information

Further information

Handle in accordance with good industrial hygiene and safety practice.

Other dangerous properties can not be excluded.

12. Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates.

EC50

Species: Daphnia magna (Water flea)

Dose: > 100 mg/l

Exposure time: 48 h

(External MSDS)

12.2 Persistence and degradability

Biodegradability

Result: Readily biodegradable.

90 - 100 %

Exposure time: 14 d

(External MSDS)

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,57

Method: (calculated)

Bioaccumulation is not expected (log Pow <1). (Lit.)

12.4 Mobility in soil

Distribution among environmental compartments

log Koc: 1,0

Method: (calculated)

Mobility of the substance in soil is expected (log koc <3). (External MSDS)

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

Do not allow to run into surface waters, wastewater, or soil.

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.

14. Transport information

Not classified as dangerous in the meaning of transport regulations.

SAFETY DATA SHEET
according to Regulation (EC) No. 1907/2006

Catalogue No. 806914
Product name (R)-(-)-Mandelic acid for resolution of racemates for synthesis

15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC
Legislation Directive 96/82/EC does not apply

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

National legislation

Storage class VCI 10 - 13 Other liquids and solids

15.2 Chemical Safety Assessment

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

16. Other information

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

H318 Causes serious eye damage.

Full text of R-phrases referred to under sections 2 and 3

R41 Risk of serious damage to eyes.

Training advice

Provide adequate information, instruction and training for operators.

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

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.

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.