

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 15.02.2018

Version 3.4

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

### 1.1 Product identifier

Catalogue No. 816011

Product name (S)-(-)-Phenylalanine 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. 63-91-2

### 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](http://www.merckgroup.com)).

### 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](mailto: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

This substance is not classified as dangerous according to European Union legislation.

### 2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

### 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> (Hill)
EC-No.	200-568-1
Molar mass	165,19 g/mol

Remarks	No disclosure requirement according to Regulation (EC) No. 1907/2006
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### 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.

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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 symptoms of toxicity.

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

Fire may cause evolution of:

nitrogen oxides

### 5.3 Advice for firefighters

*Special protective equipment for firefighters*

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

*Further information*

Suppress (knock down) gases/vapours/mists with a water spray jet. 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.

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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. 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.

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## 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).

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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)).

## *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.

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

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

Form	solid
Colour	white
Odour	weak
Odour Threshold	No information available.
pH	5,4 - 6,0 at 10 g/l 20 °C

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Melting point	275 - 283 °C (decomposition)
Boiling point/boiling range	Not applicable
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	The product is not flammable.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	< 1 Pa at 25 °C (calculated)
Relative vapour density	5,71
Density	1,34 g/cm <sup>3</sup> at 20 °C Method: OECD Test Guideline 109
Relative density	No information available.
Water solubility	27 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: -1,38 (experimental) (Lit.) Bioaccumulation is not expected.

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Auto-ignition temperature	Method: Relative self-ignition temperature for solids does not ignite
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Decomposition temperature	above melting point
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Viscosity, dynamic	No information available.
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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## 9.2 Other data

Bulk density	ca.580 kg/m <sup>3</sup>
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Particle size	Mean particle size 169 µm Method: OECD Test Guideline 110
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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.

### 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:

Strong oxidizing agents

### 10.4 Conditions to avoid



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Strong heating (decomposition).

## 10.5 Incompatible materials

no information available

## 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 oral toxicity*

LD50 Rat: 16.000 mg/kg

(ECHA)

#### *Acute inhalation toxicity*

This information is not available.

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

In vitro study

Result: No skin irritation

OECD Test Guideline 439

#### *Eye irritation*

Result: No eye irritation

Hen's egg-membrane test for irritation (HET-CAM)

#### *Sensitisation*

This information is not available.

#### *Germ cell mutagenicity*

#### *Genotoxicity in vitro*

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

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Essential amino acid.

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*

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

Analytical monitoring: yes

OECD Test Guideline 202

#### *Toxicity to algae*

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

Analytical monitoring: yes

OECD Test Guideline 201

### 12.2 Persistence and degradability

No information available.

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## 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: -1,38

(experimental)

(Lit.) 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

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.
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### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.
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### Sea transport (IMDG)

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**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*

Major Accident Hazard	SEVESO III
Legislation	Not applicable

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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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).
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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

### 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.*