

## Chemical Safety Data Sheet MSDS / SDS

**(S)-(-)-1-Phenylethyl isocyanate**

Revision Date:2023-11-29 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : (S)-(-)-1-Phenylethyl isocyanate  
CBnumber : CB5264397  
CAS : 14649-03-7  
EINECS Number : 238-698-6  
Synonyms : (S)-(-)-1-phenylethyl isocyanate,(S)-1-phenylethylisocyanate

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P501 Dispose of contents/container to.....

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P370+P378 In case of fire: Use ... for extinction.

P310 Immediately call a POISON CENTER or doctor/physician.

P309 IF exposed or if you feel unwell:

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

Continuerinsing.

P284 Wear respiratory protection.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P271 Use only outdoors or in a well-ventilated area.  
P270 Do not eat, drink or smoke when using this product.  
P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

#### **Hazard statements**

H335 May cause respiratory irritation  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H331 Toxic if inhaled  
H330 Fatal if inhaled  
H319 Causes serious eye irritation  
H315 Causes skin irritation  
H302 Harmful if swallowed  
H227 Combustible liquid

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## **SECTION 3: Composition/information on ingredients**

### **Substance**

Product name	: (S)-(-)-1-Phenylethyl isocyanate
Synonyms	: (S)-(-)-1-phenylethyl isocyanate,(S)-1-phenylethylisocyanate
CAS	: 14649-03-7
EC number	: 238-698-6
MF	: C <sub>9</sub> H <sub>9</sub> NO
MW	: 147.17

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## **SECTION 4: First aid measures**

### **Description of first aid measures**

#### **General advice**

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### **In case of skin contact**

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

#### **In case of eye contact**

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

#### **If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### **Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 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.

### Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NO<sub>x</sub>) Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.

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

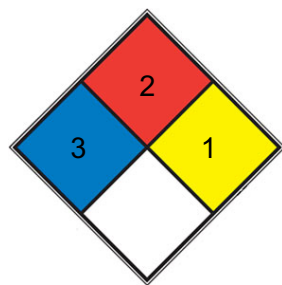
### Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 2 Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

■ REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

□ SPEC.

□ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### Environmental precautions

Do not let product enter drains.

### 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 carefully with liquid-absorbent material (e.g.

Chemizorb?). Dispose of properly. Clean up affected area.

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

#### Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

#### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### Hygiene measures

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

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

#### Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### Storage stability

Recommended storage temperature 2 - 8 °C

#### 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

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Personal protective equipment

##### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### Skin protection

required

##### Body Protection

protective clothing

##### Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type ABEK

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.

#### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	pungent
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	65 °C
Initial boiling point and boiling range	55 - 56 °C at 3,3 hPa - lit.
Flash point	65 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available

Relative density	1,045 g/cm <sup>3</sup> at 20 °C - lit. No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

## SECTION 10: Stability and reactivity

### Reactivity

Forms explosive mixtures with air on intense heating.

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

### Chemical stability

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

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat.

Strong heating.

### Incompatible materials

Alcohols, Strong bases, Amines, acids, Strong oxidizing agents, Water

### Hazardous decomposition products

In the event of fire: see section 5

## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

Oral

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 0,51 mg/l (Expert judgment)

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 0,51 mg/l (Expert judgment)

Dermal

#### Skin corrosion/irritation

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

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## SECTION 12: Ecological information

### Toxicity

**Toxicity to fish**

LC50 - Pimephales promelas (fathead minnow) - 17 mg/l - 96 h

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### Waste treatment methods

## Product

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

### UN number

ADR/RID: 2206 IMDG: 2206 IATA: 2206

### UN proper shipping name

ADR/RID: ISOCYANATES, TOXIC, N.O.S. ((S)-(-)-1-phenylethyl isocyanate) IMDG: ISOCYANATES, TOXIC, N.O.S. ((S)-(-)-1-phenylethyl isocyanate) IATA: Isocyanates, toxic, n.o.s. ((S)-(-)-1-phenylethyl isocyanate)

### Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

### Packaging group

ADR/RID: III IMDG: III IATA: III

### Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

### Special precautions for user

No data available

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## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

EC Inventory:Listed.

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

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## SECTION 16: Other information



## Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.