

## Chemical Safety Data Sheet MSDS / SDS

**(R)-(+)-1-Phenylethyl isocyanate**

Revision Date:2023-12-07 Revision Number:1

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

Product name : (R)-(+)-1-Phenylethyl isocyanate  
CBnumber : CB3212905  
CAS : 33375-06-3  
EINECS Number : 251-485-2  
Synonyms : (R)-(+)-1-phenylethyl isocyanate,(R)-(+)- $\alpha$ -methylbenzyl isocyanate

**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**

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P284 Wear respiratory protection.

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

Continuerinsing.

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

**Hazard statements**

H227 Combustible liquid

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H330 Fatal if inhaled

H331 Toxic if inhaled

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H335 May cause respiratory irritation

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: (R)-(+)-1-Phenylethyl isocyanate
Synonyms	: (R)-(+)-1-phenylethyl isocyanate,(R)-(+)- $\alpha$ -methylbenzyl isocyanate
CAS	: 33375-06-3
EC number	: 251-485-2
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

#### 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

Carbon dioxide (CO<sub>2</sub>) Dry powder

## Unsuitable extinguishing media

Foam Water

## Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx)

Hydrogen cyanide (hydrocyanic acid) 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.

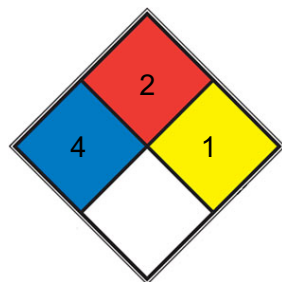
## Advice for firefighters

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 4** Very short exposure could cause death or major residual injury (e.g. hydrogen cyanide, phosgene, methyl isocyanate, [hydrofluoric 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.

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## 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.

Chemisorb?). 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

Hygroscopic. Store under inert gas. Moisture sensitive.

#### **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

## **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

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Splash contact

Material: Fluorinated rubber Minimum layer thickness: 0,7 mm Break through time: 30 min

Material tested: Vitoject? (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter B-(P2)

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	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	No data available
Initial boiling point and boiling range	55 - 56 °C at 3,3 hPa
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	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

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## 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

Exothermic reaction with:

Water Alcohols Amines alkalines

Oxidizing agents acids

### Conditions to avoid

Strong heating.

### Incompatible materials

No data available

### Hazardous decomposition products

In the event of fire: see section 5

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## 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**

No data available

**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. ((R)-(+)-1-phenylethyl isocyanate) IMDG: ISOCYANATES, TOXIC, N.O.S. ((R)-(+)-1-phenylethyl isocyanate) IATA: Isocyanates, toxic, n.o.s. ((R)-(+)-1-phenylethyl isocyanate)

### Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

### Packaging group

ADR/RID: II IMDG: II IATA: II

### 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

EC Inventory:Listed.

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

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

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

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

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

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

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

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## SECTION 16: Other information

### Abbreviations and acronyms



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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

## 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.