

## SAFETY DATA SHEET

Version 6.11  
Revision Date 04/28/2025  
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## SECTION 1. IDENTIFICATION

## 1.1 Product identifiers

Product name : (R)-(+)- $\alpha$ -Methylbenzyl isocyanate

Product Number : 77968  
Brand : Sigma-Aldrich  
CAS-No. : 33375-06-3

## 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

## 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

Flammable liquids : Category 4

Acute toxicity  
(Inhalation) : Category 2

Skin irritation : Category 2

Eye irritation : Category 2A

Respiratory sensitization : Category 1

Skin sensitization : Category 1

Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms : 

Signal Word : Danger

Hazard Statements : H227 Combustible liquid.  
H315 Causes skin irritation.  
H317 May cause an allergic skin reaction.  
H319 Causes serious eye irritation.  
H330 Fatal if inhaled.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H335 May cause respiratory irritation.

Precautionary Statements : **Prevention:**  
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P272 Contaminated work clothing must not be allowed out of the workplace.  
P280 Wear protective gloves/ eye protection/ face protection.  
P284 Wear respiratory protection.

**Response:**  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P337 + P313 If eye irritation persists: Get medical advice/ attention.  
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.  
P362 Take off contaminated clothing and wash before reuse.  
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

#### Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.  
P405 Store locked up.

#### Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

#### Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(R)-(+)-1-phenylethyl isocyanate	33375-06-3*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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### SECTION 4. 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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	: Carbon dioxide (CO <sub>2</sub> ) Dry powder
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Unsuitable extinguishing media	: Foam Water
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Specific hazards during fire fighting	: Combustible.
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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.

Hazardous combustion products	: Carbon oxides
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Nitrogen oxides (NO<sub>x</sub>)

Hydrogen cyanide (hydrocyanic acid)

Specific extinguishing methods	: No data available
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.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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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. Advice for emergency responders: 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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	: Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on	: Tightly closed.

storage conditions	Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage class	: 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
Recommended storage temperature	: 36 - 46 °F / 2 - 8 °C
Further information on storage stability	: Hygroscopic. Store under inert gas. Moisture sensitive.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

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 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.

### Hand protection

Material : butyl-rubber  
Break through time : 480 min  
Glove thickness : 0.7 mm  
Protective index : Full contact  
Manufacturer : Butoject® (KCL 898)

Material : Latex gloves  
Break through time : 10 min  
Glove thickness : 0.6 mm  
Protective index : Splash contact  
Manufacturer : Lapren® (KCL 706 / Aldrich Z677558, Size M)

Remarks	: 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: <a href="http://www.kcl.de">www.kcl.de</a> ).
Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	: protective clothing
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: clear, liquid
Color	: colorless
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point	: No data available
Boiling point/boiling range	: 131 - 133 °F / 55 - 56 °C (3.3 hPa) Method: lit.
Flash point	: 149 °F / 65 °C  Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit /	: No data available

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Upper flammability limit	
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapor density	: No data available
Relative density	: No data available
Density	: 1.046 g/cm <sup>3</sup> (68 °F / 20 °C)
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 147.17 g/mol
Particle characteristics Particle size	: 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

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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

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 0.51 mg/l - vapor

(Expert judgment)

Dermal: No data available

No data available

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

Remarks: No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### 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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## 11.2 Additional Information

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, prolonged or repeated exposure can cause:, Dizziness, Lung irritation, chest pain, pulmonary edema, Repeated exposure may cause asthma., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **(R)-(+)-1-phenylethyl isocyanate:**

Toxicity to fish : Remarks: No data available

### Persistence and degradability

#### Components:

##### **(R)-(+)-1-phenylethyl isocyanate:**

Biodegradability : Remarks: No data available

### Bioaccumulative potential

No data available

### Mobility in soil

No data available

### Other adverse effects

#### Components:

##### **(R)-(+)-1-phenylethyl isocyanate:**

Additional ecological information : No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

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**IATA-DGR**

UN/ID No. : UN 2206  
Proper shipping name : Isocyanates, toxic, n.o.s.  
((R)-(+)-1-phenylethyl isocyanate)  
Class : 6.1  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo : 662  
aircraft)  
Packing instruction : 654  
(passenger aircraft)

**IMDG-Code**

UN number : UN 2206  
Proper shipping name : ISOCYANATES, TOXIC, N.O.S.  
((R)-(+)-1-phenylethyl isocyanate)  
Class : 6.1  
Packing group : II  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : no

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National regulation****49 CFR Road**

UN/ID/NA number : UN 2206  
Proper shipping name : Isocyanates, toxic, n.o.s.  
((R)-(+)-1-phenylethyl isocyanate)  
Class : 6.1  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
ERG Code : 155  
Marine pollutant : no

Poison Inhalation Hazard : No

**Special precautions for user**

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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**SECTION 15. REGULATORY INFORMATION****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

## **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

## **US State Regulations**

### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

## **The ingredients of this product are reported in the following inventories:**

**TSCA** : Product contains substance(s) not listed on TSCA inventory.

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory

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concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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