

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

**Product Description:** (S)-(-)-a-Methylbenzyl isocyanate  
**Cat No. :** 205310000; 205310050  
**Synonyms** Ethyl isocyanate, 1-phenyl-, (S)-(-)-  
**CAS No** 14649-03-7  
**Molecular Formula** C9 H9 N O

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

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

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

#### Company

**UK entity/business name**  
 Fisher Scientific UK  
 Bishop Meadow Road,  
 Loughborough, Leicestershire LE11 5RG, United Kingdom

**EU entity/business name**  
 Thermo Fisher Scientific  
 Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

**E-mail address** begel.sdsdesk@thermofisher.com

### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

Acute Inhalation Toxicity - Dusts and Mists

Category 2 (H330)

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Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 2 (H315)  
Category 2 (H319)  
Category 3 (H335)

**Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Danger

### Hazard Statements

H319 - Causes serious eye irritation  
H330 - Fatal if inhaled  
H315 - Causes skin irritation  
H335 - May cause respiratory irritation  
Combustible liquid

### Precautionary Statements

P310 - Immediately call a POISON CENTER or doctor/physician  
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P280 - Wear protective gloves/protective clothing/eye protection/face 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

## 2.3. Other hazards

Lachrymator (substance which increases the flow of tears)  
This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
S-(-)-.alpha.-Methylbenzyl isocyanate	14649-03-7	EEC No. 238-698-6	98	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 2 (H330)

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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.
<b>Skin Contact</b>	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.
<b>Ingestion</b>	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.
<b>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

### 4.2. Most important symptoms and effects, both acute and delayed

Difficulty in breathing. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

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

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water mist may be used to cool closed containers.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

### 5.2. Special hazards arising from the substance or mixture

Combustible material. Containers may explode when heated.

#### **Hazardous Combustion Products**

Hydrogen chloride gas.

### 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

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## 6.1. Personal precautions, protective equipment and emergency procedures

Remove all sources of ignition. Take precautionary measures against static discharges.

## 6.2. Environmental precautions

See Section 12 for additional Ecological Information.

## 6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition.

## 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Keep away from open flames, hot surfaces and sources of ignition.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

### 7.2. Conditions for safe storage, including any incompatibilities

Keep refrigerated. Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 6.1A  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

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## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

#### Skin and body protection

Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

#### Respiratory Protection

Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

#### Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

#### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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## 9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Clear	
Odor	Odorless	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	55 - 56 °C / 131 - 132.8 °F	@ 2.5 mmHg
Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	65 °C / 149 °F	<b>Method -</b> No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	decomposes	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No information available	
Density / Specific Gravity	1.050	
Bulk Density	Not applicable	Liquid
Vapor Density	5.08	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

## 9.2. Other information

Molecular Formula	C9 H9 N O
Molecular Weight	147.18
Explosive Properties	explosive air/vapour mixtures possible

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions. Moisture sensitive.

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	No information available.

### 10.4. Conditions to avoid

Exposure to moisture. Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

Acids.

### 10.6. Hazardous decomposition products

Hydrogen chloride gas.

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## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

(a) acute toxicity;

Oral	No data available
Dermal	No data available
Inhalation	Category 2

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system.

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

**Symptoms / effects, both acute and delayed**

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing.

### 11.2. Information on other hazards

**Endocrine Disrupting Properties**

Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

**Ecotoxicity effects**

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

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## 12.2. Persistence and degradability

### **Persistence**

Persistence is unlikely, based on information available.

## 12.3. Bioaccumulative potential

Bioaccumulation is unlikely

## 12.4. Mobility in soil

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air

## 12.5. Results of PBT and vPvB assessment

No data available for assessment.

## 12.6. Endocrine disrupting properties

### **Endocrine Disruptor Information**

This product does not contain any known or suspected endocrine disruptors

## 12.7. Other adverse effects **Persistent Organic Pollutant** **Ozone Depletion Potential**

This product does not contain any known or suspected substance

This product does not contain any known or suspected substance

## **SECTION 13: DISPOSAL CONSIDERATIONS**

### 13.1. Waste treatment methods

#### **Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

#### **Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

#### **European Waste Catalogue (EWC)**

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### **Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## **SECTION 14: TRANSPORT INFORMATION**

### IMDG/IMO

#### 14.1. UN number

UN2206

#### 14.2. UN proper shipping name

Isocyanates, toxic, n.o.s.

#### 14.3. Transport hazard class(es)

6.1

#### 14.4. Packing group

II

### ADR



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**14.1. UN number** UN2206  
**14.2. UN proper shipping name** Isocyanates, toxic, n.o.s.  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** II

**IATA**

**14.1. UN number** UN2206  
**14.2. UN proper shipping name** ISOCYANATES, TOXIC, N.O.S.\*  
**14.3. Transport hazard class(es)** 6.1  
**14.4. Packing group** II

**14.5. Environmental hazards** No hazards identified  
**14.6. Special precautions for user** No special precautions required.  
**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

**International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
S-(-)-.alpha.-Methylbenzyl isocyanate	14649-03-7	238-698-6	-	-	-	X	-	-	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
S-(-)-.alpha.-Methylbenzyl isocyanate	14649-03-7	-	-	-	-	-	X	X

**Legend:** X - Listed '-' - Not Listed **KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**Authorisation/Restrictions according to EU REACH** Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
S-(-)-.alpha.-Methylbenzyl isocyanate	14649-03-7	-	-	-

**Seveso III Directive (2012/18/EC)**

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
S-(-)-.alpha.-Methylbenzyl isocyanate	14649-03-7	Not applicable	Not applicable

**Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals**

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Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

## National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** Water endangering class = 3 (self classification)

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
S-(-)-.alpha.-Methylbenzyl isocyanate 14649-03-7 ( 98 )	Prohibited and Restricted Substances		

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H330 - Fatal if inhaled

H335 - May cause respiratory irritation

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

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**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/MDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

## Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

## Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Revision Date** 27-Sep-2023

**Revision Summary** Not applicable.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**