

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

### 1.1. Product identifier

Product Description: 3,5-Bis(trifluoromethyl)phenyl isocyanate  
Cat No. : 314170000; 314170050  
CAS No 16588-74-2  
Molecular Formula C<sub>9</sub> H<sub>3</sub> F<sub>6</sub> 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 oral toxicity	Category 4 (H302)
Acute dermal toxicity	Category 4 (H312)

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

Acute Inhalation Toxicity - Dusts and Mists  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 4 (H332)  
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

Warning

## **Hazard Statements**

H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H315 - Causes skin irritation  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled  
Combustible liquid

## **Precautionary Statements**

P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
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
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2		98	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312)

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

				Acute Tox. 4 (H332)
--	--	--	--	---------------------

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. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
<b>Ingestion</b>	Clean mouth with water. Get medical attention.
<b>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
<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. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

### 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 spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical foam. 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. Flammable. Containers may explode when heated.

#### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Gaseous hydrogen fluoride (HF).

### 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

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## **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**

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. 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 in a dry, cool and well-ventilated place. Keep container tightly closed. Keep under nitrogen. 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 10  
**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

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## 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

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

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

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
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.

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

Physical State	Liquid	
Appearance	Colorless	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	62 °C / 143.6 °F	@ 2 mmHg
Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	67 °C / 152.6 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.470	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

### 9.2. Other information

Molecular Formula	C9 H3 F6 N O
Molecular Weight	255.12
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

Moisture sensitive.

### 10.3. Possibility of hazardous reactions

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

### 10.4. Conditions to avoid

Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines.

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## 10.6. Hazardous decomposition products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Gaseous hydrogen fluoride (HF).

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

(a) acute toxicity;

Oral	Category 4
Dermal	Category 4
Inhalation	Category 4

(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.

### 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

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## 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.

## 12.2. Persistence and degradability

### **Persistence**

No information available

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

III



# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

## ADR

**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** III

## IATA

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

**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
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	-	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	-	-	-	-	-	-	-

**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)
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	-	-	-

#### 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
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	Not applicable	Not applicable

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

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

Not applicable

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

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
3,5-Bis(trifluoromethyl)phenyl isocyanate (CAS #: 16588-74-2)	-	-	Listed	Listed	-

## PFAS Legend

Listed = Meets the PFAS definition of the named authority

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)

## 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

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H332 - Harmful 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/NDL** - 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

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

# SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)phenyl isocyanate

Revision Date 29-Sep-2023

**DNEL** - Derived No Effect Level  
**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

Predicted No Effect Concentration (PNEC)  
**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**IMO/IMDG** - 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** 29-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**