

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Creation Date 16-Nov-2010

Revision Date 29-Sep-2023

Revision Number 6

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

1.1. Product identifier

Product Description: Cat No. : CAS No Molecular Formula 3,5-Bis(trifluoromethyl)phenyl isothiocyanate 319520000; 319520010 23165-29-9 C9 H3 F6 N S

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 Pharmaceuticalaan 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 Acute dermal toxicity Category 4 (H302) Category 4 (H312)

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

Revision Date 29-Sep-2023

Acute Inhalation Toxicity - Vapors Skin Corrosion/Irritation Serious Eye Damage/Eye Irritation Category 4 (H332) Category 1 C (H314) Category 1 (H318)

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

H314 - Causes severe skin burns and eye damage

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements

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

P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting

P310 - Immediately call a POISON CENTER or doctor/physician

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

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

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 isothiocyanate	23165-29-9		>95	Skin Corr. 1C (H314) Eye Dam. 1 (H318) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice	Immediate medical attention is required. Show this safety data sheet to the doctor in attendance.
Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Get medical attention.
Inhalation	Remove to fresh air. Get medical attention. If not breathing, give artificial respiration.
Self-Protection of the First Aider	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

Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

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

CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons No information available.

5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

Hazardous Combustion Products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulfur oxides.

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. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6: ACCIDENTAL RELEASE MEASURES

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

6.1. Personal precautions, protective equipment and emergency procedures

Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Use personal protective equipment as required. Ensure adequate ventilation.

6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material.

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

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Avoid contact with skin, eyes or clothing. Avoid breathing dust/fume/gas/mist/vapors/spray. Avoid ingestion and inhalation.

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

Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 8A 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

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

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

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

Nitrile rubber	Breakthrough time See manufacturers recommendations	Glove thickness -	EU standard EN 374	Glove comments (minimum requirement)
Skin and body protect	tion Long sle	eved 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 compatability, 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.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance Odor Odor Threshold Melting Point/Range Softening Point Boiling Point/Range Flammability (liquid) Flammability (solid,gas) Explosion Limits	Yellow No information available No data available No data available 63 °C / 145.4 °F No data available Not applicable No data available	@ 1.5 mmHg Liquid
Flash Point Autoignition Temperature Decomposition Temperature pH Viscosity Water Solubility Solubility in other solvents Partition Coefficient (n-octanol/wate	No information available No data available No data available No information available No data available No information available No information available	Method - No information available
Vapor Pressure Density / Specific Gravity Bulk Density Vapor Density Particle characteristics	No data available No data available Not applicable No data available Not applicable (liquid)	Liquid (Air = 1.0)
9.2. Other information		
Molecular Formula	C9 H3 F6 N S	

271.18

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
10.2. Chemical stability	Stable under normal conditions.
10.3. Possibility of hazardous react	ions
Hazardous Polymerization Hazardous Reactions	Hazardous polymerization does not occur. None under normal processing.
10.4. Conditions to avoid	Incompatible products. Excess heat. Exposure to moist air or water.
10.5. Incompatible materials	Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides.

SECTION 11: TOXICOLOGICAL INFORMATION

Molecular Weight

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

Product Information	
(a) acute toxicity; Oral Dermal Inhalation	Category 4 Category 4 Category 4
(b) skin corrosion/irritation;	Category 1 C
(c) serious eye damage/irritation;	Category 1
(d) respiratory or skin sensitization; Respiratory Skin	No data available 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;	No data available
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
Symptoms / effects,both acute and delayed	Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.
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.

12.2. Persistence and degradability Persistence	No information available Persistence is unlikely, based on information available.		
12.3. Bioaccumulative potential	Bioaccumulation is unlikely		
<u>12.4. Mobility in soil</u>	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		
<u>12.5. Results of PBT and vPvB</u> assessment	No data available for assessment.		
<u>12.6. Endocrine disrupting</u> 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		
SE	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. Do not flush to sewer. Large amounts will affect pH and harm aquatic organisms.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN1760
14.2. UN proper shipping name	Corrosive liquid, n.o.s.
14.3. Transport hazard class(es)	8
14.4. Packing group	III

<u>ADR</u>

<u>14.1. UN number</u> 14.2. UN proper shipping name UN1760 Corrosive liquid, n.o.s.

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

14.3. Transport hazard class(es)	8
14.4. Packing group	III

IATA

<u>14.1. UN number</u> <u>14.2. UN proper shipping name</u> <u>14.3. Transport hazard class(es)</u> <u>14.4. Packing group</u>	UN1760 Corrosive liquid, n.o.s. 8 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	23165-29-9	-	-	-	-	Х	-	-	-
isothiocyanate									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3,5-Bis(trifluoromethyl)phenyl isothiocyanate	23165-29-9	-	-	-	-	-	-	-

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	0	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3,5-Bis(trifluoromethyl)phenyl isothiocyanate	23165-29-9	-	-	-

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)pheny I isothiocyanate	23165-29-9	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

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	-	-	Listed	Listed	-
isothiocyanate					
(CAS #: 23165-29-9)					

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

H332 - Harmful if inhaled

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

Legend

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
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	NZIOC - New Zealand Inventory of Chemicals
WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Governmental Industrial Hygienists	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	Predicted No Effect Concentration (PNEC)
RPE - Respiratory Protective Equipment	LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%	EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol:Water
PBT - Persistent, Bioaccumulative, Toxic	vPvB - very Persistent, very Bioaccumulative

Ships

Transport Association

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

3,5-Bis(trifluoromethyl)phenyl isothiocyanate

Revision Date 29-Sep-2023

ICAO/IATA - International Civil Aviation Organization/International Air

MARPOL - International Convention for the Prevention of Pollution from

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

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.

Creation Date	16-Nov-2010
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