

# SAFETY DATA SHEET

Revision Date 19-Dec-2025

Revision Number 5

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

## 1. Identification

**Product Name** 3,5-Bis(trifluoromethyl)phenyl isocyanate

**Cat No. :** AC314170000; AC314170010; AC314170050

**CAS No** 16588-74-2  
**Synonyms** No information available

**Recommended Use** Laboratory chemicals.  
**Uses advised against** Food, drug, pesticide or biocidal product use.

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

#### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

#### **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

## 2. Hazard(s) identification

### Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

Flammable liquids	Category 4
Acute oral toxicity	Category 4
Acute dermal toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

### Label Elements

#### **Signal Word**

Warning

**Hazard Statements**

Combustible liquid  
Causes skin irritation  
Causes serious eye irritation  
May cause respiratory irritation  
Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling  
Do not eat, drink or smoke when using this product  
Wear protective gloves/protective clothing/eye protection/face protection  
Avoid breathing dust/fume/gas/mist/vapors/spray  
Use only outdoors or in a well-ventilated area  
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
Keep cool

**Inhalation**

IF INHALED: Remove person to fresh air and keep comfortable for breathing  
Call a POISON CENTER or doctor if you feel unwell

**Skin**

IF ON SKIN: Wash with plenty of soap and water  
Call a POISON CENTER or doctor if you feel unwell  
If skin irritation occurs: Get medical advice/attention  
Take off contaminated clothing

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
If eye irritation persists: Get medical advice/attention

**Ingestion**

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell  
Rinse mouth

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam to extinguish

**Storage**

Store in a well-ventilated place. Keep container tightly closed  
Store locked up

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

None identified

**Hazards classified under paragraph (d)(1)(ii) of 1910.1200**

No information available

### 3. Composition/information on Ingredients

Component	CAS No	Weight %
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	<=100

#### 4. 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>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.
<b>Ingestion</b>	Clean mouth with water. Get medical attention.
<b>Most important symptoms and effects</b>	Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
<b>Notes to Physician</b>	Treat symptomatically

#### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Water spray. Carbon dioxide (CO <sub>2</sub> ). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	67 °C / 152.6 °F
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	No information available
<b>Explosion Limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

#### Specific Hazards Arising from the Chemical

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).

#### Protective Equipment and Precautions for Firefighters

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

#### NFPA

**Health**  
2

**Flammability**  
1

**Instability**  
0

**Physical hazards**  
N/A

#### 6. Accidental release measures

<b>Personal Precautions</b>	Remove all sources of ignition. Take precautionary measures against static discharges.
<b>Environmental Precautions</b>	See Section 12 for additional Ecological Information.
<b>Methods for Containment and Clean Up</b>	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.

#### 7. Handling and Storage

<b>Handling</b>	Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Use spark-proof tools
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and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition.

**Storage.**

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

## 8. Exposure controls / personal protection

**Exposure Guidelines**

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

**Engineering Measures**

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

**Personal Protective Equipment****Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin and body protection**

Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection**

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 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.

**Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

**Appearance****Physical State**

Liquid

**Color**

Colorless

**Odor**

No information available

**Odor Threshold**

No information available

**Property****Values****Remarks****• Method****Melting Point/Range**

No data available

**Softening Point**

No data available

**Boiling Point/Range**

62 °C / 143.6 °F

@ 2 mmHg

**Flash Point**

67 °C / 152.6 °F

**Method -** No information available

**Flammability (liquid)**

Combustible liquid

On basis of test data

**Flammability (solid,gas)**

Not applicable

Liquid

**Explosion Limits**

No data 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

<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

**Other Information**

<b>Molecular Formula</b>	C9 H3 F6 N O
<b>Molecular Weight</b>	255.12
<b>Explosive Properties</b>	explosive air/vapour mixtures possible

## 10. Stability and reactivity

<b>Reactive Hazard</b>	None known, based on information available
<b>Stability</b>	Moisture sensitive.
<b>Conditions to Avoid</b>	Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.
<b>Incompatible Materials</b>	Acids, Strong oxidizing agents, Strong bases, Alcohols, Amines
<b>Hazardous Decomposition Products</b>	Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Gaseous hydrogen fluoride (HF)
<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

**Information on expected route of exposure**

<b>Inhalation</b>	Not an expected route of exposure.
<b>Ingestion</b>	May be harmful if swallowed.
<b>Eyes</b>	Lachrymator (substance which increases the flow of tears). Avoid contact with eyes. Irritating to eyes.
<b>Skin</b>	Harmful in contact with skin. Avoid contact with skin. May cause irritation.

**Toxicology data for the components**

<b>Toxicologically Synergistic Products</b>	No information available
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**(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;**

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	Not listed	Not listed	Not listed	Not listed	Not listed

(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.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

## 12. Ecological information

### Ecotoxicity

Do not empty into drains.

Persistence and Degradability Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its volatility.

## 13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

### DOT

UN-No UN2206  
 Proper Shipping Name Isocyanates, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group III

### TDG

UN-No UN2206  
 Proper Shipping Name Isocyanate solution, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group III

### IATA

UN-No UN2206  
 Proper Shipping Name Isocyanate solution, toxic, n.o.s.  
 Hazard Class 6.1  
 Packing Group III

**IMDG/IMO**

<b>UN-No</b>	UN2206
<b>Proper Shipping Name</b>	Isocyanates, toxic, n.o.s.
<b>Hazard Class</b>	6.1
<b>Packing Group</b>	III

**15. Regulatory Information****United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	-	-	-

**Legend:****TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

**TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)**

Not applicable

**TSCA 12(b)** - Notices of Export

Not applicable

**International Inventories**

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	-	-	-	-	-		-	-	-

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)**U.S. Federal Regulations****SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

**SARA 311/312 Hazard Categories**

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

**CWA (Clean Water Act)**

Not applicable

**Clean Air Act**

Not applicable

**OSHA** - Occupational Safety and Health Administration

Not applicable

**CERCLA**

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations** Not applicable

**U.S. Department of Transportation**

Reportable Quantity (RQ): N

DOT Marine Pollutant N

DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**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	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	Not applicable	Not applicable	Not applicable	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

**Other International Regulations**

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
3,5-Bis(trifluoromethyl)phenyl isocyanate	16588-74-2	Not applicable	Not applicable	Not applicable	Not applicable

**16. Other Information**



<b>Prepared By</b>	Product stewardship (Regulatory Affairs) Thermo Fisher Scientific email - begel.sdsdesk@thermofisher.com
<b>Revision Date</b>	19-Dec-2025
<b>Print Date</b>	19-Dec-2025
<b>Revision Summary</b>	Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

**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 SDS**