

## SAFETY DATA SHEET

Creation Date 23-October-2010

Revision Date 01-September-2023

Revision Number 5

### 1. Identification

**Product Name** 4-(Trifluoromethoxy)phenyl isocyanate

**Cat No. :** SB01053DA; SB01053EA; SB01053EB; SB01053ZZ

**CAS-No** 35037-73-1

**Synonyms** 1-Isocyanato-4-(trifluoromethoxy)benzene

**Recommended Use** Laboratory chemicals.

**Uses advised against** Food, drug, pesticide or biocidal product use.

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

##### Company

**Importer/Distributor**  
Fisher Scientific  
112 Colonnade Road,  
Ottawa, ON K2E 7L6,  
Canada  
Tel: 1-800-234-7437

Fisher Scientific  
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

**WHMIS 2015 Classification** Classified as hazardous under the Hazardous Products Regulations (SOR/2015-17)

<b>Flammable liquids</b>	Category 4
<b>Acute oral toxicity</b>	Category 4
<b>Acute dermal toxicity</b>	Category 3
<b>Acute Inhalation Toxicity</b>	Category 1
<b>Skin Corrosion/Irritation</b>	Category 1 C
<b>Serious Eye Damage/Eye Irritation</b>	Category 1
<b>Respiratory Sensitization</b>	Category 1
<b>Skin Sensitization</b>	Category 1
<b>Specific target organ toxicity (single exposure)</b>	Category 3
Target Organs - Respiratory system.	

#### Label Elements

**Signal Word**

Danger

#### Hazard Statements

Combustible liquid  
 Harmful if swallowed  
 Toxic in contact with skin  
 Fatal if inhaled  
 Causes severe skin burns and eye damage  
 May cause an allergic skin reaction  
 May cause allergy or asthma symptoms or breathing difficulties if inhaled  
 May cause respiratory irritation



#### Precautionary Statements

##### Prevention

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
 Do not breathe dust/fumes/gas/mist/vapours/spray  
 Wash face, hands and any exposed skin thoroughly after handling  
 Do not eat, drink or smoke when using this product  
 Use only outdoors or in a well-ventilated area  
 Contaminated work clothing should not be allowed out of the workplace  
 Wear protective gloves/protective clothing/eye protection/face protection  
 Wear respiratory protection

##### Response

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower  
 IF INHALED: Remove person to fresh air and keep comfortable for breathing  
 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
 Immediately call a POISON CENTER/doctor  
 Rinse mouth  
 Do NOT induce vomiting  
 Wash contaminated clothing before reuse  
 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

##### Storage

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

##### Disposal

Dispose of contents/container to an approved waste disposal plant

#### Other Hazards

Harmful to aquatic life with long lasting effects

### 3. Composition/Information on Ingredients

Component	CAS-No	Weight %
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	>95

### 4. First-aid measures

#### General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Remove to fresh air. Immediate medical attention is required.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately.
<b>Most important symptoms/effects</b>	Causes burns by all exposure routes. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. 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: 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
<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, alcohol-resistant foam. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	No information available
<b>Flash Point</b>	69 °C / 156.2 °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

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Combustible material. Containers may explode when heated.

### Hazardous Combustion Products

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid). 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. Thermal decomposition can lead to release of irritating gases and vapors.

### NFPA

<b>Health</b>	<b>Flammability</b>	<b>Instability</b>	<b>Physical hazards</b>
4	2	0	N/A

## 6. Accidental release measures

<b>Personal Precautions</b>	Ensure adequate ventilation. Use personal protective equipment as required. Evacuate
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**Environmental Precautions** personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges. Should not be released into the environment. Do not flush into surface water or sanitary sewer system.

**Methods for Containment and Clean Up** Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition.

## 7. Handling and storage

**Handling** Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition.

**Storage.** Keep in a dry place. Keep container tightly closed. Keep away from heat, sparks and flame. Store under an inert atmosphere. Keep refrigerated. Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents. Alcohols. Amines. Water.

## 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. 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  
**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	Glove comments
Nitrile rubber	See manufacturers recommendations	-	Splash protection only
Neoprene			
Natural rubber			
PVC			

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) 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. gloves with care avoiding skin contamination.

### **Respiratory Protection**

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

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

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

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

### **Environmental exposure controls**

Prevent product from entering drains.

**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.

## 9. Physical and chemical properties

<b>Physical State</b>	Liquid
<b>Appearance</b>	Clear
<b>Odor</b>	No information available
<b>Odor Threshold</b>	No information available
<b>pH</b>	No information available
<b>Melting Point/Range</b>	No data available
<b>Boiling Point/Range</b>	78 °C / 172.4 °F @ 22 mmHg
<b>Flash Point</b>	69 °C / 156.2 °F
<b>Evaporation Rate</b>	No information available
<b>Flammability (solid,gas)</b>	Not applicable
<b>Flammability or explosive limits</b>	
<b>Upper</b>	No data available
<b>Lower</b>	No data available
<b>Vapor Pressure</b>	No information available
<b>Vapor Density</b>	7.0
<b>Specific Gravity</b>	1.340
<b>Solubility</b>	No information available
<b>Partition coefficient; n-octanol/water</b>	No data available
<b>Autoignition Temperature</b>	No information available
<b>Decomposition Temperature</b>	No information available
<b>Viscosity</b>	No information available
<b>Molecular Formula</b>	C8 H4 F3 N O2
<b>Molecular Weight</b>	203.12
<b>Refractive index</b>	1.457-1.460

## 10. Stability and reactivity

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

## 11. Toxicological information

**Acute Toxicity**
**Product Information**  
**Component Information**

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	Not listed	LD50 = 670 mg/kg ( Rat ) LD50 = 268 mg/kg ( Rat )	LC50 22.5 - 68.5 mg/m <sup>3</sup> ( Rat ) 4 h

**Toxicologically Synergistic Products** No information available

**Delayed and immediate effects as well as chronic effects from short and long-term exposure**

**Irritation** No information available

**Sensitization** May cause sensitization by skin contact

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

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	Not listed	Not listed	Not listed	Not listed	Not listed

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** Respiratory system

**STOT - repeated exposure** None known

**Aspiration hazard** No information 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: 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

**Endocrine Disruptor Information** No information available

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

## 12. Ecological information

### Ecotoxicity

Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

**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** UN3390  
**Proper Shipping Name** TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.  
**Technical Name** Benzene, 1-isocyanato-4-(trifluoromethoxy)-

<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I
<b>TDG</b>	
<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I
<b>IATA</b>	
	FORBIDDEN FOR IATA TRANSPORT
<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.* FORBIDDEN FOR IATA TRANSPORT
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I
<b>IMDG/IMO</b>	
<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I

## 15. Regulatory information

### International Inventories

Component	CAS-No	DSL	NDSL	TSCA	TSCA Inventory notification - Active-Inactive	EINECS	ELINCS	NLP
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	-	X	X	ACTIVE	252-328-0	-	-

Component	CAS-No	IECSC	KECL	ENCS	ISHL	TCSI	AICS	NZIoC	PICCS
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	-	-	-	-	X	-	-	-

#### Legend:

X - Listed '-' - Not Listed

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

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

**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

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

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

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

**AICS** - Australian Inventory of Chemical Substances

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

### Canada

SDS in compliance with provisions of information as set out in Canadian Standard - Part 4, Schedule 1 and 2 of the Hazardous Products Regulations (HPR) and meets the requirements of the HPR (Paragraph 13(1)(a) of the Hazardous Products Act (HPA)).

### Other International Regulations

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

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

Component	CAS-No	OECD HPV	Persistent Organic	Ozone Depletion	Restriction of

			Pollutant	Potential	Hazardous Substances (RoHS)
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	Not applicable	Not applicable	Not applicable	Not applicable

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)
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	35037-73-1	Not applicable	Not applicable	Not applicable	Not applicable

## 16. Other information

<b>Prepared By</b>	Regulatory Affairs Thermo Fisher Scientific Email: EMSDS.RA@thermofisher.com
<b>Creation Date</b>	23-October-2010
<b>Revision Date</b>	01-September-2023
<b>Print Date</b>	01-September-2023
<b>Revision Summary</b>	This document has been updated to comply with the requirements of WHMIS 2015 to align with the Globally Harmonised System (GHS) for the Classification and Labelling of Chemicals.

### 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**