

ALFAAB20033

## 4-(Trifluoromethoxy)phenyl isocyanate

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

**产品说明:**  
**Product Description:** 4-三氟甲氧基苯基异氰酸酯  
 4-(Trifluoromethoxy)phenyl isocyanate

**Cat No. :** B20033  
**Synonyms** 1-Isocyanato-4-(trifluoromethoxy)benzene  
**CAS No** 35037-73-1  
**Molecular Formula** C8 H4 F3 N O2

**Supplier** Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
 Shore Road, Heysham  
 Lancashire, LA3 2XY,  
 United Kingdom  
 Office Tel: +44 (0) 1524 850506  
 Office Fax: +44 (0) 1524 850608

**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

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

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

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Liquid

**Appearance**  
Clear

**Odor**  
No information available

#### Emergency Overview

Combustible liquid. Harmful if swallowed. Toxic in contact with skin. Causes severe skin burns and eye damage. May cause an allergic skin reaction. Fatal if inhaled. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Harmful to aquatic life with long lasting effects. Moisture sensitive. Lachrymator (substance which increases the flow of tears).

#### Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 1 C
Serious Eye Damage/Eye Irritation	Category 1
Respiratory Sensitization	Category 1
Skin Sensitization	Category 1
Specific target organ toxicity - (single exposure)	Category 3
Chronic aquatic toxicity	Category 3

#### Label Elements

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

**Signal Word****Danger****Hazard Statements**

H227 - Combustible liquid  
H302 - Harmful if swallowed  
H311 - Toxic in contact with skin  
H314 - Causes severe skin burns and eye damage  
H317 - May cause an allergic skin reaction  
H330 - Fatal if inhaled  
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H335 - May cause respiratory irritation  
H412 - Harmful to aquatic life with long lasting effects

**Precautionary Statements****Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P270 - Do not eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P272 - Contaminated work clothing should not be allowed out of the workplace  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P284 - In case of inadequate ventilation wear respiratory protection

**Response**

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P310 - Immediately call a POISON CENTER or doctor  
P330 - Rinse mouth  
P331 - Do NOT induce vomiting  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

Harmful if swallowed. Toxic in contact with skin. Corrosive. Causes skin and eye burns. May cause an allergic skin reaction. Fatal if inhaled. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

**Environmental hazards**

Harmful to aquatic life with long lasting effects. Will likely be mobile in the environment due to its volatility. The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces.

**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**

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

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

### SECTION 4. FIRST AID MEASURES

#### General Advice

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

#### Eye Contact

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.

#### Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

#### Inhalation

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.

#### Ingestion

Do NOT induce vomiting. Call a physician or poison control center immediately.

#### Most important symptoms and effects

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

#### 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.

#### Notes to Physician

Treat symptomatically.

### SECTION 5. FIRE-FIGHTING MEASURES

#### Suitable Extinguishing Media

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

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

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.

#### 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.

### SECTION 6. ACCIDENTAL RELEASE MEASURES

#### Personal Precautions

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges.

### Environmental Precautions

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.

Refer to protective measures listed in Sections 8 and 13.

## SECTION 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.

### Specific Use(s)

Use in laboratories

## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Control Parameters

### Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

### 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				

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)

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

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.

<b>Skin and body protection</b>	Long sleeved clothing
<b>Respiratory Protection</b>	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
<b>Large scale/emergency use</b>	Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced <b>Recommended Filter type:</b> Organic gases and vapours filter Type A Brown conforming to EN14387
<b>Small scale/Laboratory use</b>	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. <b>Recommended half mask:-</b> Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141 When RPE is used a face piece Fit Test should be conducted
<b>Hygiene Measures</b>	Handle in accordance with good industrial hygiene and safety practice.
<b>Environmental exposure controls</b>	Prevent product from entering drains.

### SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>	Clear	
<b>Physical State</b>	Liquid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</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>Method -</b> No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	7.0	(Air = 1.0)
<b>Specific Gravity / Density</b>	1.340	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	No data available	
<b>Explosive Properties</b>		explosive air/vapour mixtures possible
<b>Oxidizing Properties</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	

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

### SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Stable. Moisture sensitive.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<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>Materials to avoid</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).

### SECTION 11. TOXICOLOGICAL INFORMATION

#### Product Information

##### (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Benzene, 1-isocyanato-4-(trifluoromethoxy)-		LD50 = 670 mg/kg ( Rat ) LD50 = 268 mg/kg ( Rat )	LC50 22.5 - 68.5 mg/m <sup>3</sup> ( Rat ) 4 h

(b) skin corrosion/irritation; Category 1 C

(c) serious eye damage/irritation; Category 1

##### (d) respiratory or skin sensitization;

Respiratory

Category 1

Skin

Category 1

May cause sensitization by skin contact

(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

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

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

### SECTION 12. ECOLOGICAL INFORMATION

<b>Ecotoxicity effects</b>	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.
<b>Persistence and Degradability</b> <b>Persistence</b> <b>Degradation in sewage treatment plant</b>	No information available Persistence is unlikely, based on information available. Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.
<b>Bioaccumulative Potential</b>	Bioaccumulation is unlikely
<b>Mobility in soil</b>	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.
<b>Endocrine Disruptor Information</b> <b>Persistent Organic Pollutant</b> <b>Ozone Depletion Potential</b>	This product does not contain any known or suspected endocrine disruptors This product does not contain any known or suspected substance This product does not contain any known or suspected substance

### SECTION 13. DISPOSAL CONSIDERATIONS

<b>Waste from Residues/Unused Products</b>	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.
<b>Contaminated Packaging</b>	Dispose of this container to hazardous or special waste collection point.
<b>Other Information</b>	Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Large amounts will affect pH and harm aquatic organisms. Do not let this chemical enter the environment.

### SECTION 14. TRANSPORT INFORMATION

#### Road and Rail Transport

<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Technical Shipping Name</b>	4-(Trifluoromethoxy)phenyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8
<b>Packing Group</b>	I

#### IMDG/IMO

<b>UN-No</b>	UN3390
<b>Proper Shipping Name</b>	TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.
<b>Technical Shipping Name</b>	4-(Trifluoromethoxy)phenyl isocyanate
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	8

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

Packing Group I

IATA FORBIDDEN FOR IATA TRANSPORT

UN-No UN3390  
 Proper Shipping Name TOXIC BY INHALATION LIQUID, CORROSIVE, N.O.S.\* FORBIDDEN FOR IATA TRANSPORT  
 Technical Shipping Name 4-(Trifluoromethoxy)phenyl isocyanate  
 Hazard Class 6.1  
 Subsidiary Hazard Class 8  
 Packing Group I

Special Precautions for User No special precautions required

### SECTION 15. REGULATORY INFORMATION

#### International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Benzene, 1-isocyanato-4-(trifluoromethoxy)-	-	-	X	-	252-328-0	X	-	-	-		-	-

#### National Regulations

### SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department  
 Creation Date 23-Oct-2010  
 Revision Date 22-Apr-2024  
 Revision Summary New emergency telephone response service provider.

#### 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.

#### 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

# SAFETY DATA SHEET

## 4-(Trifluoromethoxy)phenyl isocyanate

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

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association  
**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road  
**OECD** - Organisation for Economic Co-operation and Development  
**BCF** - Bioconcentration factor

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

### 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**