

ALFAAL11890

4-(Trifluoromethyl)phenyl isothiocyanate

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

产品说明: 4-三氟甲基苯基硫代异氰酸酯
Product Description: 4-(Trifluoromethyl)phenyl isothiocyanate

Cat No. : L11890
CAS No 1645-65-4
Molecular Formula C8 H4 F3 NS

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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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
Solid

Appearance
White

Odor
pungent

Emergency Overview

Harmful in contact with skin. Causes skin irritation. Lachrymator (substance which increases the flow of tears). Harmful if swallowed. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation.

Classification of the substance or mixture

| | |
|--|------------|
| Acute Oral Toxicity | Category 4 |
| Acute Dermal Toxicity | Category 4 |
| Acute Inhalation Toxicity - Dusts and Mists | Category 4 |
| Skin Corrosion/Irritation | Category 2 |
| Serious Eye Damage/Eye Irritation | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |

Label Elements



Signal Word**Warning****Hazard Statements**

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

Precautionary Statements**Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
 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
 P280 - Wear protective gloves/protective clothing/eye protection/face protection

Response

P312 - Call a POISON CENTER or doctor if you feel unwell
 P330 - Rinse mouth
 P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
 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
 P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

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

Disposal

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

Physical and Chemical Hazards

None identified.

Health Hazards

Harmful in contact with skin. Causes skin irritation. Harmful if swallowed. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants.

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

| Component | CAS No | Weight % |
|--|-----------|----------|
| 4-(Trifluoromethyl)phenyl isothiocyanate | 1645-65-4 | <=100 |

SECTION 4. FIRST AID MEASURES
General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

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Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

Most important symptoms and effects

None reasonably foreseeable.

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

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

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.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

Environmental Precautions

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

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

Storage

Keep container tightly closed in a dry and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

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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. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

Exposure Controls**Engineering Measures**

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 recommendations | - | EN 374 | (minimum requirement) |
| Neoprene | | | | |
| 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)

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.

Skin and body protection Long sleeved clothing

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: Particulates filter conforming to EN 143

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:- Particle filtering: EN149:2001
When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance White
Physical State Solid

Odor pungent
Odor Threshold No data available
pH No information available

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| | | |
|--|-------------------------------|--|
| Melting Point/Range | 39 - 42 °C / 102.2 - 107.6 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 207 °C / 404.6 °F | |
| Flash Point | > 110 °C / > 230 °F | Method - No information available |
| Evaporation Rate | Not applicable | Solid |
| Flammability (solid,gas) | No information available | |
| Explosion Limits | No data available | |
| Vapor Pressure | No data available | |
| Vapor Density | Not applicable | Solid |
| Specific Gravity / Density | No data available | |
| Bulk Density | No data available | |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| Viscosity | Not applicable | Solid |
| Explosive Properties | No information available | |
| Oxidizing Properties | No information available | |
| Molecular Formula | C8 H4 F3 NS | |
| Molecular Weight | 203.19 | |

SECTION 10. STABILITY AND REACTIVITY

| | |
|---|-----------------------------------|
| Stability | Stable under normal conditions. |
| Hazardous Reactions | None under normal processing. |
| Hazardous Polymerization | No information available. |
| Conditions to Avoid | None known. |
| Materials to avoid | No information available. |
| Hazardous Decomposition Products | None under normal use conditions. |

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

| | |
|---|---|
| (a) acute toxicity; | |
| (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 |

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| | |
|--|---------------------------|
| (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; | Not applicable Solid |
| Symptoms / effects,both acute and delayed | No information available |

SECTION 12. ECOLOGICAL INFORMATION

| | |
|--|---|
| Ecotoxicity effects | Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants. |
| Persistence and Degradability | No information available |
| Bioaccumulative Potential | No information available |
| Mobility in soil | No information available |
| Endocrine Disruptor Information | This product does not contain any known or suspected endocrine disruptors |
| Persistent Organic Pollutant | This product does not contain any known or suspected substance |
| Ozone Depletion Potential | This product does not contain any known or suspected substance |

SECTION 13. DISPOSAL CONSIDERATIONS

| | |
|--|--|
| 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. |
| 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

Road and Rail Transport

| | |
|--------------------------------|--|
| UN-No | UN2923 |
| Proper Shipping Name | Corrosive solid, toxic, n.o.s. |
| Technical Shipping Name | (4-(Trifluoromethyl)phenyl isothiocyanate) |
| Hazard Class | 8 |
| Subsidiary Hazard Class | 6.1 |

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Packing Group III

IMDG/IMO

UN-No UN2923
Proper Shipping Name Corrosive solid, toxic, n.o.s.
Technical Shipping Name (4-(Trifluoromethyl)phenyl isothiocyanate)
Hazard Class 8
Subsidiary Hazard Class 6.1
Packing Group III

IATA

UN-No UN2923
Proper Shipping Name CORROSIVE SOLID, TOXIC, N.O.S.*
Technical Shipping Name (4-(Trifluoromethyl)phenyl isothiocyanate)
Hazard Class 8
Subsidiary Hazard Class 6.1
Packing Group III

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 |
|--|---|---|------|-------|--------|------|-----|-------|------|------|------|------|
| 4-(Trifluoromethyl)phenyl isothiocyanate | - | - | X | - | - | - | - | - | - | | - | - |

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 19-Sep-2025
Revision Summary Not applicable.

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

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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

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

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

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