

ALFAAL11646

3-(Trifluoromethyl)phenyl isothiocyanate

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

| | |
|--------------------------------------|--|
| 产品说明: Product Description: | 3-(三氟甲基)苯基硫代异氰酸酯, 98% 3-(Trifluoromethyl)phenyl isothiocyanate |
| Cat No. : | L11646 |
| Synonyms | 3-Trifluoromethylphenylisothiocyanate |
| CAS No | 1840-19-3 |
| Molecular Formula | C8 H4 F3 N S |
| 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 Yellow-orange | Odor No information available |
| Emergency Overview | | |
| Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Moisture sensitive. | | |

Classification of the substance or mixture

| | |
|--|------------|
| 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 |

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**

P264 - Wash face, hands and any exposed skin thoroughly after handling
 P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
 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

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
 P312 - Call a POISON CENTER or doctor if you feel unwell
 P330 - Rinse mouth
 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 if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation.

Environmental hazards

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

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | CAS No | Weight % |
|--|-----------|----------|
| alpha,alpha,alpha-Trifluoro-m-tolyl isothiocyanate | 1840-19-3 | 98 |

SECTION 4. FIRST AID MEASURES

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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

Inhalation

SAFETY DATA SHEET

3-(Trifluoromethyl)phenyl isothiocyanate

Remove from exposure, lie down. Remove to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Get medical attention.

Ingestion

Clean mouth with water. Get medical attention.

Most important symptoms and effects

No information available.

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 (CO₂). Dry chemical. Chemical foam.

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.

Environmental Precautions

See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Do not let this chemical enter the environment.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

Handling

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Control Parameters

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 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 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.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

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

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 Yellow-orange
Physical State Liquid

Odor No information available

SAFETY DATA SHEET

3-(Trifluoromethyl)phenyl isothiocyanate

| | | |
|--|---------------------------------|--|
| Odor Threshold | No data available | |
| pH | No information available | |
| Melting Point/Range | No data available | |
| Softening Point | No data available | |
| Boiling Point/Range | 206 - 208 °C / 402.8 - 406.4 °F | |
| Flash Point | 94 °C / 201.2 °F | Method - No information available |
| Evaporation Rate | No data available | |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Vapor Pressure | No data available | |
| Vapor Density | 7.01 | (Air = 1.0) |
| Specific Gravity / Density | 1.335 | |
| Bulk Density | Not applicable | Liquid |
| 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 | No data available | |
| Explosive Properties | No information available | |
| Oxidizing Properties | No information available | |
| Molecular Formula | C8 H4 F3 N S | |
| Molecular Weight | 203.19 | |

SECTION 10. STABILITY AND REACTIVITY

| | |
|---|---|
| Stability | Moisture sensitive. |
| Hazardous Reactions | No information available. |
| Hazardous Polymerization | No information available. |
| Conditions to Avoid | Incompatible products. Exposure to moist air or water. |
| Materials to avoid | Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines. Strong reducing agents. |
| Hazardous Decomposition Products | Carbon monoxide (CO). Carbon dioxide (CO ₂). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF). |

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 |

SAFETY DATA SHEET

3-(Trifluoromethyl)phenyl isothiocyanate

| | |
|--|--|
| (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 |
| Other Adverse Effects | The toxicological properties have not been fully investigated. |
| Symptoms / effects,both acute and delayed | No information available |

SECTION 12. ECOLOGICAL INFORMATION

| | |
|--|---|
| Ecotoxicity effects | Do not empty into drains. |
| 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 | UN2810 |
| Proper Shipping Name | Toxic liquid, organic, n.o.s. |
| Hazard Class | 6.1 |

SAFETY DATA SHEET

3-(Trifluoromethyl)phenyl isothiocyanate

Packing Group II

IMDG/IMO

UN-No UN2810
Proper Shipping Name Toxic liquid, organic, n.o.s.
Hazard Class 6.1
Packing Group II

IATA

UN-No UN2810
Proper Shipping Name TOXIC LIQUID, ORGANIC, N.O.S.*
Hazard Class 6.1
Packing Group II

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 |
|--|---|---|------|-------|--------|------|-----|-------|------|------|------|------|
| alpha,alpha,alpha-Trifluoro-m-tolyl isothiocyanate | - | - | X | - | - | - | - | - | - | | - | - |

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 25-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

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

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

PICCS - Philippines Inventory of Chemicals and Chemical Substances

ENCS - Japanese Existing and New Chemical Substances

SAFETY DATA SHEET

3-(Trifluoromethyl)phenyl isothiocyanate

IECSC - Chinese Inventory of Existing Chemical Substances
KECL - Korean Existing and Evaluated Chemical Substances

AICS - Australian Inventory of Chemical Substances
NZIoC - New Zealand Inventory of Chemicals

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

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End of Safety Data Sheet