**SAFETY DATA SHEET**

**4-(Trifluoromethyl)phenyl isocyanate**

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

**Product Description:** 4-(Trifluoromethyl)phenyl isocyanate

**Cat No.:** L12576

**CAS No:** 1548-13-6

**Molecular Formula:** C8 H4 F3 N O

**Supplier**

Alfa Aesar
Avocado Research Chemicals, Ltd.
Shore Road
Port of Heysham Industrial Park
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**Emergency Telephone Number**

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+44 (0) 1235 239670 (Multi-language)

**E-mail address**

uktech@alfa.com
www.alfa.com
Product Safety Department

**Recommended Use**

Laboratory chemicals,

**Uses advised against**

No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Classification of the substance or mixture**

<table>
<thead>
<tr>
<th>Flammable liquids.</th>
<th>Category 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Oral Toxicity</td>
<td>Category 4</td>
</tr>
<tr>
<td>Acute Dermal Toxicity</td>
<td>Category 4</td>
</tr>
<tr>
<td>Acute Inhalation Toxicity - Vapors</td>
<td>Category 2</td>
</tr>
<tr>
<td>Skin Corrosion/Irritation</td>
<td>Category 2</td>
</tr>
<tr>
<td>Serious Eye Damage/Eye Irritation</td>
<td>Category 2</td>
</tr>
<tr>
<td>Respiratory Sensitization</td>
<td>Category 1</td>
</tr>
<tr>
<td>Specific target organ toxicity - (single exposure)</td>
<td>Category 3</td>
</tr>
</tbody>
</table>

**Label Elements**

**Physical State**

Liquid

**Appearance**

Colorless

**Odor**

No information available

**Emergency Overview**

Combustible liquid. Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Fatal if inhaled. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Moisture sensitive. Lachrymator (substance which increases the flow of tears).
Signal Word  Danger

Hazard Statements
H227 - Combustible liquid
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H330 - Fatal if inhaled
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335 - May cause respiratory irritation
H302 + H312 - Harmful if swallowed or in contact with skin

Precautionary Statements
Prevention
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P271 - Use only outdoors or in a well-ventilated area
P264 - Wash face, hands and any exposed skin thoroughly after handling
P270 - Do not eat, drink or smoke when using this product
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P284 - In case of inadequate ventilation wear respiratory 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
P310 - Immediately call a POISON CENTER or doctor/physician
P330 - Rinse mouth
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. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. 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
Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. 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)

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS No</th>
<th>Weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-Trifluoromethoxyphenyl isocyanate</td>
<td>1548-13-6</td>
<td>99</td>
</tr>
</tbody>
</table>
SECTION 4. FIRST AID MEASURES

Eye Contact
Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact
Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required.

Inhalation
Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required.

Ingestion
Call a physician immediately. Clean mouth with water.

Most important symptoms and effects
Difficulty in breathing. May cause allergy or asthma symptoms or breathing difficulties if inhaled. 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

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
Carbon dioxide (CO\textsubscript{2}). Dry chemical. 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
Combustible material. Flammable. 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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal Precautions
Remove all sources of ignition. Take precautionary measures against static discharges.

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. Wear self-contained breathing apparatus and protective suit. Do not let this chemical enter the environment. Remove all sources of ignition.
Handling
Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation. Keep away from open flames, hot surfaces and sources of ignition.

Storage

Specific Use(s)
Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

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 |

<table>
<thead>
<tr>
<th>Glove material</th>
<th>Breakthrough time</th>
<th>Glove thickness</th>
<th>EU standard</th>
<th>Glove comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrile rubber</td>
<td>See manufacturers</td>
<td>-</td>
<td>EN 374</td>
<td>(minimum requirement)</td>
</tr>
<tr>
<td>Neoprene</td>
<td>recommendations</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Natural rubber</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PVC</td>
<td></td>
<td></td>
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</tbody>
</table>

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**

Colorless

**Physical State**

Liquid

**Odor**

No information available

**Odor Threshold**

No data available

**pH**

No information available

**Melting Point/Range**

No data available

**Softening Point**

No data available

**Boiling Point/Range**

58 - 59 °C / 136.4 - 138.2 °F @ 10 mmHg

**Flash Point**

69 °C / 156.2 °F Method - No information available

**Evaporation Rate**

No data available

**Flammability (solid,gas)**

Not applicable

**Explosion Limits**

No data available

**Vapor Pressure**

No data available

**Vapor Density**

No data available

**Specific Gravity / Density**

1.310 (Air = 1.0)

**Bulk Density**

Not applicable Liquid

**Water Solubility**

No information available

**Solubility in other solvents**

No information available

**Partition Coefficient (n-octanol/water)**

No data available

**Autoignition Temperature**

No data available

**Decomposition Temperature**

No data available

**Viscosity**

No data available

**Explosive Properties**

No information available explosive air/vapour mixtures possible

**Oxidizing Properties**

No information available

**Molecular Formula**

C8 H4 F3 N O

**Molecular Weight**

187.12

**SECTION 10. STABILITY AND REACTIVITY**

**Stability**

Moisture sensitive.

**Hazardous Reactions**

No information available.

**Hazardous Polymerization**

Hazardous polymerization does not occur.

**Conditions to Avoid**

Excess heat. Incompatible products. Exposure to moist air or water. Keep away from open flames, hot surfaces and sources of ignition.
Materials to avoid

Hazardous Decomposition Products

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 Category 1
   Skin No data available
   No information available
(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

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

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects
Do not empty into drains.

Persistence and Degradability
Persistence
No information available
Persistence is unlikely, based on information available.

Bioaccumulative Potential
Bioaccumulation is unlikely
Mobility in soil

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.

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

UN3382

Proper Shipping Name

TOXIC BY INHALATION LIQUID, N.O.S.

Technical Shipping Name

α,α,α-Trifluoro-p-tolyl isocyanate

Hazard Class

6.1

Packing Group

I

IMDG/IMO

UN-No

UN3382

Proper Shipping Name

TOXIC BY INHALATION LIQUID, N.O.S.

Technical Shipping Name

α,α,α-Trifluoro-p-tolyl isocyanate

Hazard Class

6.1

Packing Group

I

IATA

FORBIDDEN FOR IATA TRANSPORT

UN-No

UN3382

Proper Shipping Name

TOXIC BY INHALATION LIQUID, N.O.S. FORBIDDEN FOR IATA TRANSPORT

Technical Shipping Name

α,α,α-Trifluoro-p-tolyl isocyanate

Hazard Class

6.1

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).

<table>
<thead>
<tr>
<th>Component</th>
<th>The Inventory of Hazardous Chemicals (2015)</th>
<th>List of dangerous goods GB 12268 - 2012</th>
<th>TCSI</th>
<th>IECSC</th>
<th>EINECS</th>
<th>TSCA</th>
<th>DSL</th>
<th>PICCS</th>
<th>ENCS</th>
<th>ISHL</th>
<th>AICS</th>
<th>KECL</th>
</tr>
</thead>
</table>
National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 06-Jan-2023
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
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
IIECS - 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
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
OECD - Organisation for Economic Co-operation and Development
BCF - Bioconcentration factor
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
WEL - Workplace Exposure Limit
TWA - Time Weighted Average
IARC - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)
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
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