

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

1.1. Product identifier

Product Description:	<u>4-(Trifluoromethyl)phenyl isocyanate</u>
Cat No. :	L12576
CAS No	1548-13-6
Molecular Formula	C ₈ H ₄ F ₃ N O
REACH registration number	-

1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

1.3. Details of the supplier of the safety data sheet

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

1.4. 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

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity

Category 4 (H302)

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Acute dermal toxicity
Acute Inhalation Toxicity - Dusts and Mists
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Respiratory Sensitization
Specific target organ toxicity - (single exposure)

Category 4 (H312)
Category 2 (H330)
Category 2 (H315)
Category 2 (H319)
Category 1 (H334)
Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

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

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P310 - Immediately call a POISON CENTER or doctor/physician
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P342 + P311 - If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician
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
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. 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

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
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3-Trifluoromethylphenyl isocyanate	1548-13-6	EEC No. 216-284-6	99	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Resp. Sens. 1 (H334) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 2 (H330)
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REACH registration number	-
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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.
Ingestion	Call a physician immediately. Clean mouth with water.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required.
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.

4.2. Most important symptoms and effects, both acute and delayed

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

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician	Treat symptomatically.
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SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Carbon dioxide (CO₂). Dry chemical. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Combustible material. Flammable. Containers may explode when heated.

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen cyanide (hydrocyanic acid), Gaseous hydrogen fluoride (HF).

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5.3. Advice 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

6.1. Personal precautions, protective equipment and emergency procedures

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

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning 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.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe 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.

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.

7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry place. Keep container tightly closed. Keep away from heat, sparks and flame. Store under an inert atmosphere. Keep refrigerated. Keep containers tightly closed in a dry, cool and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510
Storage Class (LGK) (Germany)

Class 6.1A

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

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Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. 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				

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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.

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

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Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Colorless	
Odor	No information available	
Odor Threshold	No data 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
Flammability (liquid)	Combustible liquid	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	69 °C / 156.2 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.310	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C8 H4 F3 N O
Molecular Weight	187.12
Explosive Properties	explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Moisture sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	No information available.

10.4. Conditions to avoid

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

10.5. Incompatible materials

Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines.

10.6. Hazardous decomposition products

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Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid). Gaseous hydrogen fluoride (HF).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information

(a) acute toxicity;

Oral	Category 4
Dermal	Category 4
Inhalation	Category 2

(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.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

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12.1. Toxicity

Ecotoxicity effects Do not empty into drains.

12.2. Persistence and degradability

Persistence

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

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

12.4. 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.

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

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.

European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

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

IMDG/IMO

14.1. UN number

UN3382

14.2. UN proper shipping name

TOXIC BY INHALATION LIQUID, N.O.S.

Technical Shipping Name

α,α,α -Trifluoro-p-tolyl isocyanate

14.3. Transport hazard class(es)

6.1

14.4. Packing group

I

ADR

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14.1. UN number UN3382
14.2. UN proper shipping name TOXIC BY INHALATION LIQUID, N.O.S.
Technical Shipping Name α,α,α -Trifluoro-p-tolyl isocyanate
14.3. Transport hazard class(es) 6.1
14.4. Packing group I

IATA FORBIDDEN FOR IATA TRANSPORT

14.1. UN number UN3382
14.2. UN proper shipping name TOXIC BY INHALATION LIQUID, N.O.S. FORBIDDEN FOR IATA TRANSPORT
Technical Shipping Name α,α,α -Trifluoro-p-tolyl isocyanate
14.3. Transport hazard class(es) 6.1
14.4. Packing group I

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
3-Trifluoromethylphenyl isocyanate	1548-13-6	216-284-6	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-Trifluoromethylphenyl isocyanate	1548-13-6	-	-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed

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

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3-Trifluoromethylphenyl isocyanate	1548-13-6	-	-	-

Seveso III Directive (2012/18/EC)

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
3-Trifluoromethylphenyl isocyanate	1548-13-6	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals
Not applicable

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Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

See table for values

Component	OECD PFAS	US (EPA) PFAS	EU (ECHA) PFAS	UK (HSE) PFAS	Chemsec PFAS (Sin List)
3-Triflouromethylphenyl isocyanate (CAS #: 1548-13-6)	-	-	Listed	Listed	-

PFAS Legend

Listed = Meets the PFAS definition of the named authority

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

Water endangering class = 3 (self classification)

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
3-Triflouromethylphenyl isocyanate 1548-13-6 (99)	Prohibited and Restricted Substances		

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

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

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

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer
Predicted No Effect Concentration (PNEC)

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RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic

LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

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

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

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.

Prepared By	Health, Safety and Environmental Department
Revision Date	07-Feb-2024
Revision Summary	New emergency telephone response service provider.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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