

ALFAAL09899

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

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

产品说明: 2-氯-5-(三氟甲基)苯基异氰酸酯
Product Description: 2-Chloro-5-(trifluoromethyl)phenyl isocyanate

Cat No. : L09899
CAS No 50528-86-4
Molecular Formula C₈ H₃ Cl F₃ N O

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
Colorless

Odor
pungent

Emergency Overview

Combustible liquid. Harmful if swallowed. Causes skin irritation. Causes serious eye irritation. Toxic 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).

Classification of the substance or mixture

| | |
|--|------------|
| Flammable liquids. | Category 4 |
| Acute Oral Toxicity | Category 4 |
| Acute Inhalation Toxicity - Vapors | Category 3 |
| Skin Corrosion/Irritation | Category 2 |
| Serious Eye Damage/Eye Irritation | Category 2 |
| Respiratory Sensitization | Category 1 |
| Specific target organ toxicity - (single exposure) | Category 3 |

Label Elements

SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

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

H227 - Combustible liquid
H302 - Harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H331 - Toxic if inhaled
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335 - May cause respiratory irritation

Precautionary Statements**Prevention**

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
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
P284 - In case of inadequate ventilation wear respiratory protection

Response

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
P311 - Call a POISON CENTER or doctor
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. Causes skin irritation. Causes serious eye irritation. Toxic 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)
This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | CAS No | Weight % |
|---|------------|----------|
| 2-Chloro-5-(trifluoromethyl)phenyl isocyanate | 50528-86-4 | <=100 |

SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

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

Remove to fresh air. 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. Immediate medical attention is required.

Ingestion

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

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

No special precautions required.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES

Suitable Extinguishing Media

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. 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

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

Environmental Precautions

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

SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

Methods for Containment and Clean Up

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. 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 refrigerated. Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame.

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

None under normal use conditions. Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. .

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)

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 Long sleeved clothing

Respiratory Protection No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particle filter

Small scale/Laboratory use

Maintain adequate ventilation

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

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 | pungent | |
| Odor Threshold | No data available | |
| pH | No information available | |
| Melting Point/Range | No data available | |
| Softening Point | No data available | |
| Boiling Point/Range | 52 - 53 °C / 125.6 - 127.4 °F | |
| Flash Point | 92 °C / 197.6 °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 | No data available | (Air = 1.0) |
| Specific Gravity / Density | 1.48 g/cm3 | @ 20 °C |
| 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 | | explosive air/vapour mixtures possible |
| Oxidizing Properties | No information available | |
| Molecular Formula | C8 H3 Cl F3 N O | |
| Molecular Weight | 221.57 | |

SECTION 10. STABILITY AND REACTIVITY

| | |
|---|---|
| Stability | Stable under normal conditions. |
| Hazardous Reactions | None under normal processing. |
| Hazardous Polymerization | No information available. |
| Conditions to Avoid | Keep away from open flames, hot surfaces and sources of ignition. |
| Materials to avoid | No information available. |
| Hazardous Decomposition Products | None under normal use conditions. |

SECTION 11. TOXICOLOGICAL INFORMATION

SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

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

(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 of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

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
Persistence 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

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

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 UN2206
Proper Shipping Name Isocyanates, toxic, n.o.s.
Technical Shipping Name (2-Chloro-5-(trifluoromethyl)phenyl isocyanate)
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN2206
Proper Shipping Name Isocyanates, toxic, n.o.s.
Technical Shipping Name (2-Chloro-5-(trifluoromethyl)phenyl isocyanate)
Hazard Class 6.1
Packing Group III

IATA

UN-No UN2206
Proper Shipping Name ISOCYANATES, TOXIC, N.O.S.*
Technical Shipping Name (2-Chloro-5-(trifluoromethyl)phenyl isocyanate)
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 |
|---|---|---|------|-------|--------|------|-----|-------|------|------|------|------|
| 2-Chloro-5-(trifluoromethyl)phenyl isocyanate | - | - | X | - | - | - | - | - | - | - | - | - |

National Regulations

SAFETY DATA SHEET

2-Chloro-5-(trifluoromethyl)phenyl isocyanate

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 03-May-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.

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

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