

# SAFETY DATA SHEET

according to the OSHA  
Hazard Communication Standard

Version 7.0  
Revision Date 04/17/2026  
Print Date 04/18/2026

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 4-Chloro-3-(trifluoromethyl)phenyl  
isocyanate

Product Number : 374881  
Brand : Aldrich  
CAS-No. : 327-78-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

Acute toxicity (Oral)	: Category 4
Acute toxicity (Inhalation)	: Category 4
Acute toxicity (Dermal)	: Category 4
Skin irritation	: Category 2
Serious eye damage	: Category 1
Respiratory sensitisation	: Category 1
Skin sensitisation	: Category 1
Specific target organ toxicity - single exposure	: Category 3 (Respiratory system)

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.  
H315 Causes skin irritation.  
H317 May cause an allergic skin reaction.  
H318 Causes serious eye damage.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H335 May cause respiratory irritation.

Precautionary statements : **Prevention:**  
P261 Avoid breathing dust.  
P264 Wash 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.  
P272 Contaminated work clothing must not be allowed

out of the workplace.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P285 In case of inadequate ventilation wear respiratory protection.

**Response:**

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P302 + P352 + P312 IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.

P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.

**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.

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 327-78-6

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
3-Trifluoromethyl-4-chlorophenyl isocyanate	327-78-6*	>= 80 - <= 100	TSC

\* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

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**SECTION 4. FIRST AID MEASURES**

General advice	: First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.
If inhaled	: After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.
In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products	: Carbon oxides  Nitrogen oxides (NOx)  Hydrogen chloride gas  Hydrogen fluoride
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
- Further information on storage conditions : Tightly closed.  
Dry.  
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 11, Combustible Solids
- Recommended storage temperature : Recommended storage temperature see product label.
- Further information on storage stability : Moisture sensitive.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection  
Material : Nitrile rubber

Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Full contact
Manufacturer	: Dermatril® (KCL 740 / Aldrich Z677272, Size M)
Material	: Nitrile rubber
Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Splash contact
Manufacturer	: Dermatril® (KCL 740 / Aldrich Z677272, Size M)
Remarks	: This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: <a href="http://www.kcl.de">www.kcl.de</a> ).
Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles
Skin and body protection	: protective clothing
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: powder
Color	: white
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 104 - 108 °F / 40 - 42 °C Method: lit.
Boiling point/boiling range	: 187 - 194 °F / 86 - 90 °C (19 hPa) Method: lit.
Flash point	: 210 °F / 99 °C

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Method: closed cup

Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 221.56 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating.  A range from approx. 15 Kelvin below the flash point is to be rated as critical.  The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Strong heating.
Incompatible materials	: Strong oxidizing agents
Hazardous decomposition products	: In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### **Acute toxicity**

LD50 Oral - Rat - female - 500 mg/kg

(OECD Test Guideline 423)

Acute toxicity estimate Inhalation - Expert judgement - 4 h - 1.5 mg/l - dust/mist

Acute toxicity estimate Dermal - Expert judgement - 1,100.1 mg/kg

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: Irritating to skin. - 4 h

(OECD Test Guideline 404)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

#### **Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

May cause allergic respiratory and skin reactions

#### **Germ cell mutagenicity**

Test Type: Ames test

Test system: S. typhimurium  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative

### **Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.  
NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.  
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

No data available

### **Persistence and degradability**

No data available

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

### **Other adverse effects**

#### **Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was

manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

### **Endocrine disrupting properties**

No data available

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## **SECTION 13. DISPOSAL CONSIDERATIONS**

### **Disposal methods**

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## **SECTION 14. TRANSPORT INFORMATION**

### **International Regulations**

#### **IATA-DGR**

Not regulated as a dangerous good

#### **IMDG-Code**

Not regulated as a dangerous good

#### **Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

### **National Regulations**

#### **49 CFR**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

### **Special precautions for user**

Remarks : Not classified as dangerous in the meaning of transport regulations.

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## **SECTION 15. REGULATORY INFORMATION**

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

### **SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

### **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312** : Acute Health Hazard

## Hazards

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

## US State Regulations

### Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

### Maine Chemicals of High Concern

Product does not contain any listed chemicals

### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

### Washington Chemicals of High Concern

Product does not contain any listed chemicals

### The components of this product are reported in the following inventories:

US TSCA : Product contains substance(s) not listed on TSCA inventory.

### TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## SECTION 16. OTHER INFORMATION

### Relevant changes since previous version

8. Exposure controls/personal protection

### Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); EC<sub>x</sub> - Concentration associated with x% response; EHS - Extremely Hazardous Substance; EL<sub>x</sub> - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErC<sub>x</sub> - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC<sub>50</sub> - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC<sub>50</sub> - Lethal Concentration to 50 % of a test population; LD<sub>50</sub> - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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