SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: 4-(Trifluoromethyl)phenyl isocyanate
Product Number: 250821
Brand: Aldrich
CAS-No.: 1548-13-6

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

Identified uses: Laboratory chemicals, Synthesis of substances

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

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Respiratory sensitization (Category 1), H334
Skin sensitization (Category 1), H317
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.
2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word
Danger

Hazard statement(s)
H227 Combustible liquid.
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335 May cause respiratory irritation.

Precautionary statement(s)
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261 Avoid breathing mist or vapors.
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/ eye protection/ face protection.
P285 In case of inadequate ventilation wear respiratory protection.
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 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Lachrymator.
SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: α,α,α-Trifluoro-p-tolyl isocyanate

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>α,α,α-Trifluoro-p-tolyl isocyanate</td>
<td>Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; H227, H302, H332, H312, H315, H319, H334, H317, H335</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material 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. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed
No data available
SECTION 5: Firefighting measures

5.1 Extinguishing media

**Suitable extinguishing media**
- Water
- Foam
- Carbon dioxide (CO₂)
- Dry powder

**Unsuitable extinguishing media**
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

- Carbon oxides
- Nitrogen oxides (NOₓ)
- Hydrogen fluoride
- Combustible.
- Vapors 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.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

**Advice on safe handling**

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability
Recommended storage temperature
2 - 8 °C
Moisture sensitive. Handle and store under inert gas.

Storage class
Storage class (TRGS 510): 10: Combustible liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection
required

Body Protection
protective clothing

Respiratory protection
Recommended Filter type: Filter type ABEK
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. required when vapours/aerosols 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.

**Control of environmental exposure**
Do not let product enter drains.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: clear, liquid</td>
</tr>
<tr>
<td></td>
<td>Color: colorless</td>
</tr>
<tr>
<td>b) Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>58 - 59 °C 136 - 138 °F at 13 hPa - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>69 °C (156 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>No data available</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>m) Density</td>
<td>1.31 g/cm3 at 25 °C (77 °F) - lit.</td>
</tr>
<tr>
<td></td>
<td>Relative density</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>No data available</td>
</tr>
<tr>
<td>o) Partition coefficient: n-octanol/water</td>
<td>No data available</td>
</tr>
<tr>
<td>p) Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>t) Oxidizing properties</td>
<td>none</td>
</tr>
</tbody>
</table>
9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Heat.
Strong heating.

10.5 Incompatible materials
Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
Acute toxicity estimate Oral - Expert judgment - 500.1 mg/kg
Acute toxicity estimate Inhalation - Expert judgment - 4 h - 11.1 mg/l - vapor

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

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
IARC: No ingredient 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 ingredient 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**
Cough, Shortness of breath, Headache, Nausea, Vomiting, Repeated exposure may cause asthma., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

**SECTION 12: Ecological information**

12.1 **Toxicity**
No data available

12.2 **Persistence and degradability**
No data available

12.3 **Bioaccumulative potential**
No data available

12.4 **Mobility in soil**
No data available

12.5 **Results of PBT and vPvB assessment**
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 **Endocrine disrupting properties**
No data available

12.7 **Other adverse effects**
No data available

---

**SECTION 13: Disposal considerations**

13.1 **Waste treatment methods**

**Product**
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.
SECTION 14: Transport information

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

Further information
Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

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

SARA 313 Components
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.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

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

SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact misbranding@sigma-aldrich.com.

Version: 6.4 Revision Date: 08/01/2023 Print Date: 12/23/2023

Aldrich - 250821

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