

## SAFETY DATA SHEET

Version 4.4  
Revision Date 07/01/2014  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 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, Manufacture of substances

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

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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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 sensitisation (Category 1), H334

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.

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 dust/ fume/ gas/ mist/ vapours/ spray.
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.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P332 + P313	If skin irritation 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 or doctor/ physician.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
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.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms :  $\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate

Formula :  $C_8H_4F_3NO$   
Molecular Weight : 187.12 g/mol  
CAS-No. : 1548-13-6  
EC-No. : 216-284-6

#### Hazardous components

Component	Classification	Concentration
<b><math>\alpha,\alpha,\alpha</math>-Trifluoro-p-tolyl isocyanate</b>		
	Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; STOT SE 3; H227, H302 + H312 + H332, H315, H319, H334, H335	-

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

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**5. FIREFIGHTING MEASURES****5.1 Extinguishing media****Suitable extinguishing media**

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides, nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride

**5.3 Advice for firefighters**

Wear self contained breathing apparatus for fire fighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities**

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature: 2 - 8 °C

Moisture sensitive. Handle and store under inert gas.

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: clear, liquid<br>Colour: colourless            |
| b) Odour  | no data available                                    |
| c) Odour Threshold                              | no data available                                    |
| d) pH   | no data available                                    |
| e) Melting point/freezing point                 | no data available                                    |
| f) Initial boiling point and boiling range      | 58 - 59 °C (136 - 138 °F) at 13 hPa (10 mmHg) - lit. |
| g) Flash point                                  | 69 °C (156 °F) - closed cup                          |
| h) Evaporation rate                             | no data available                                    |
| i) Flammability (solid, gas)                    | no data available                                    |
| j) Upper/lower flammability or explosive limits | no data available                                    |
| k) Vapour pressure                              | no data available                                    |
| l) Vapour density                               | no data available                                    |
| m) Relative density                             | 1.31 g/cm <sup>3</sup> at 25 °C (77 °F)              |

- |    |  |                   |
|----|--|-------------------|
| n) | Water solubility                       | no data available |
| o) | Partition coefficient: n-octanol/water | no data available |
| p) | Auto-ignition temperature              | no data available |
| q) | Decomposition temperature              | no data available |
| r) | Viscosity                              | no data available |
| s) | Explosive properties                   | no data available |
| t) | Oxidizing properties                   | no data available |

## 9.2 Other safety information

no data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

no data available

### 10.4 Conditions to avoid

Heat.

Heat, flames and sparks.

### 10.5 Incompatible materials

Water, Alcohols, Strong bases, Amines, acids, Strong oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

no data available

no data available

#### Skin corrosion/irritation

no data available

#### Serious eye damage/eye irritation

no data available

#### Respiratory or skin sensitisation

#### Germ cell mutagenicity

no data available

#### 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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

no data available

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

**Additional Information**

RTECS: Not available

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.

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## 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 Other adverse effects

no data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

UN number: 3382 Class: 6.1

Packing group: I

Proper shipping name: Toxic by inhalation liquid, n.o.s. ( $\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate)

Marine pollutant: No

Poison Inhalation Hazard: Hazard zone B

**IMDG**

UN number: 3382 Class: 6.1

Packing group: I

EMS-No: F-A, S-A

Proper shipping name: TOXIC BY INHALATION LIQUID, N.O.S. ( $\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate)

Marine pollutant: No

**IATA**

UN number: 3382      Class: 6.1

Proper shipping name: Toxic by inhalation liquid, n.o.s. ( $\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate)

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

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**15. REGULATORY INFORMATION****SARA 302 Components**

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

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.

**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.

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
$\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate	1548-13-6	

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
$\alpha,\alpha,\alpha$ -Trifluoro-p-tolyl isocyanate	1548-13-6	

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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**16. OTHER INFORMATION****Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H227	Combustible liquid
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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