

## SAFETY DATA SHEET

Version 8.4  
Revision Date 08/06/2021  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-Chloro-4-methylphenyl isocyanate

Product Number : 478245  
Brand : Aldrich  
CAS-No. : 28479-22-3

**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)**

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  
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)	
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)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ 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 + 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.
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/ doctor.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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

Formula	: C <sub>8</sub> H <sub>6</sub> ClNO
Molecular weight	: 167.59 g/mol
CAS-No.	: 28479-22-3
EC-No.	: 249-050-7

Component	Classification	Concentration
<b>3-Chloro-4-tolyl isocyanate</b>		
	Acute Tox. 4; Acute Tox. 2; Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1;	<= 100 %

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	STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H302, H330, H312, H314, H318, H334, H317, H335, H400, H410	
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For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material 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

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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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides  
Nitrogen oxides (NO<sub>x</sub>)  
Hydrogen chloride gas

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

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**

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

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

#### **Hygiene measures**

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

For precautions see section 2.2.

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

#### **Storage conditions**

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.

#### **Storage stability**

Recommended storage temperature

2 - 8 °C

Moisture sensitive. Handle and store under inert gas.

#### **Storage class**

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

### **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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## **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

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

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |  |                                  |
|--|----------------------------------|
| a) Appearance                              | Form: liquid<br>Color: colorless |
| b) Odor                                    | No data available                |
| c) Odor Threshold                          | No data available                |
| d) pH                                      | No data available                |
| e) Melting point/freezing point            | No data available                |
| f) Initial boiling point and boiling range | 107 °C 225 °F at 4 hPa - lit.    |
| g) Flash point                             | 109 °C (228 °F) - closed cup     |
| h) Evaporation rate                        | No data available                |
| i) Flammability (solid, gas)               | No data available                |
| j) Upper/lower flammability or             | No data available                |

explosive limits

- |  |   |
|--|---|
| k) Vapor pressure                            | No data available                               |
| l) Vapor density                             | No data available                               |
| m) Density                                   | 1.224 g/cm <sup>3</sup> at 25 °C (77 °F) - lit. |
| Relative density                             | No data available                               |
| n) Water solubility                          | No data available                               |
| o) Partition coefficient:<br>n-octanol/water | No data available                               |
| p) Autoignition<br>temperature               | No data available                               |
| q) Decomposition<br>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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## SECTION 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

Avoid moisture.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 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

Acute toxicity estimate Oral - Expert judgment - 500.1 mg/kg

LC50 Inhalation - Rat - female - 4 h - 0.071 mg/l

(OECD Test Guideline 403)

Symptoms: mucosal irritations, Cough, Shortness of breath, Headache, Possible damages:, damage of respiratory tract, Inhalation may lead to the formation of oedemas in the respiratory tract.

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

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

Skin - Rabbit

Result: Causes burns. - 24 h

Remarks: (ECHA)

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

Causes serious eye damage.

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

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

Result: negative

Remarks: (ECHA)

#### **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**

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.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish

static test LC50 - *Leuciscus idus melanotus* - 47 mg/l - 96 h

Remarks: (ECHA)

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Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.62 mg/l - 48 h (DIN 38412)
Toxicity to algae	ErC50 - Scenedesmus pannonicus - 4.8 mg/l - 96 h Remarks: (ECHA)

## 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 20 d  
Result: 0 % - Not readily biodegradable.  
(OECD Test Guideline 301D)

## 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

Discharge into the environment must be avoided.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2236 Class: 6.1 Packing group: II  
Proper shipping name: 3-Chloro-4-methylphenyl isocyanate, liquid  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2236 Class: 6.1 Packing group: II EMS-No: F-A, S-A  
Proper shipping name: 3-CHLORO-4-METHYLPHENYL ISOCYANATE, LIQUID

### IATA

UN number: 2236 Class: 6.1 Packing group: II  
Proper shipping name: 3-Chloro-4-methylphenyl isocyanate, liquid

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## SECTION 15: Regulatory information

### SARA 302 Components

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

### 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

Acute Health Hazard

### Massachusetts Right To Know Components

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

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

### Pennsylvania Right To Know Components

3-Chloro-4-tolyl isocyanate	CAS-No. 28479-22-3	Revision Date 2007-03-01
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3-Chloro-4-tolyl isocyanate	CAS-No. 28479-22-3	Revision Date 2007-03-01
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### New Jersey Right To Know Components

3-Chloro-4-tolyl isocyanate	CAS-No. 28479-22-3	Revision Date 2007-03-01
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## SECTION 16: Other information

### Further information

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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](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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