

SAFETY DATA SHEET

Version 8.9
Revision Date 09/08/2024
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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

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

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 2), H330
Acute toxicity, Dermal (Category 4), H312
Skin corrosion (Category 1B), H314

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Serious eye damage (Category 1), H318
 Respiratory sensitization (Category 1), H334
 Skin sensitization (Category 1), H317
 Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
 Short-term (acute) aquatic hazard (Category 1), H400
 Long-term (chronic) aquatic hazard (Category 1), H410

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 Statements

H302 + H312

Harmful if swallowed or in contact with skin.

H314

Causes severe skin burns and eye damage.

H317

May cause an allergic skin reaction.

H330

Fatal if inhaled.

H334

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H335

May cause respiratory irritation.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P260

Do not breathe 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.

P273

Avoid release to the environment.

P280

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

P284

Wear respiratory protection.

P301 + P312 + P330

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

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

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.

P363

Wash contaminated clothing before reuse.

P391

Collect spillage.

P403 + P233

Store in a well-ventilated place. Keep container tightly closed.

P405

Store locked up.

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

Lachrymator.

SECTION 3: Composition/information on ingredients**3.1 Substances**

Formula : C_8H_6ClNO
 Molecular weight : 167.59 g/mol
 CAS-No. : 28479-22-3
 EC-No. : 249-050-7

Component	Classification	Concentration
3-Chloro-4-tolyl isocyanate		
	Acute Tox. 4; Acute Tox. 2; Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H302, H330, H312, H314, H318, H334, H317, H335, H400, H410	<= 100 %

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. Call a physician immediately.

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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Foam Water

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen chloride gas

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

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. 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.

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 in a well-ventilated place. 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): 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

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). Tightly fitting safety goggles

Skin protection

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: www.kcl.de).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatrill® L

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: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatrill® L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter B-(P3)

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 dusts/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

- | | |
|--|---|
| a) Appearance | Form: liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point: 23 °C (73 °F) - (ECHA) |
| f) Initial boiling point and boiling range | 107 °C 225 °F at 4 hPa - lit. |
| g) Flash point | 109 °C (228 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| h) Evaporation rate | No data available |

i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.224 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	1.2320 °C - Regulation (EC) No. 440/2008, Annex, A.3
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

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

Violent reactions possible with:

Water

Alcohols

Strong oxidizing agents

Amines

alkalines

acids

The generally known reaction partners of water.

10.4 Conditions to avoid

Avoid moisture.

Strong heating.

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10.5 Incompatible materials

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

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

(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

Remarks: 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.

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	static test LC50 - <i>Leuciscus idus melanotus</i> - 47 mg/l - 96 h Remarks: (ECHA)
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Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 0.62 mg/l - 48 h (DIN 38412)
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Toxicity to algae	ErC50 - <i>Scenedesmus pannonicus</i> - 4.8 mg/l - 96 h Remarks: (ECHA)
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12.2 Persistence and degradability

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

Discharge into the environment must be avoided.

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)

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

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.

US State Regulations

Massachusetts Right To Know

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

Maine Chemicals of High Concern

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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 ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the 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.

SECTION 16: Other information

Further information

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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