

SAFETY DATA SHEET

Version 6.9 Revision Date 09/19/2025 Print Date 09/20/2025

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 4-Chlorophenyl isocyanate

Product Number : 152277 Brand : Aldrich

Index-No. : 615-044-00-1 CAS-No. : 104-12-1

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

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 3

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Acute toxicity (Inhalation)

: Category 2

Skin irritation : Category 2

Serious eye damage : Category 1

Respiratory sensitisation : Category 1

Specific target organ toxicity - single exposure

Category 3 (Respiratory system)

Short-term (acute)

aquatic hazard

: Category 1

Long-term (chronic)

aquatic hazard

: Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms











Signal Word : Danger

Hazard Statements : H301 Toxic if swallowed.

H315 Causes skin irritation.

H318 Causes serious eye damage.

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 : **Prevention:**

P260 Do not breathe 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.

P273 Avoid release to the environment.

P280 Wear protective gloves/ eye protection/ face

protection.

P284 Wear respiratory protection.

Response:

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P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P352 IF ON SKIN: Wash with plenty of water. 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. P332 + P313 If skin irritation occurs: Get medical

advice/ attention. P342 + P311 If experiencing respiratory symptoms: Call

a POISON CENTER/ doctor. P391 Collect spillage.

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.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4- Chloroisocyanatobenzen e	104-12-1*	>= 80 - <= 100	TSC

^{*} Indicates that the identifier is a CAS No.

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

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

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contaminated clothing. Rinse skin with water/ shower.

In case of eye contact : After eye contact: rinse out with plenty of water.

Immediately call in ophthalmologist.

Remove contact lenses.

If swallowed : If swallowed: give water to drink (two glasses at

most). Seek medical advice immediately. In

exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and

consult a doctor as quickly as possible.

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

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing

media

: Water

Foam

Carbon dioxide (CO2)

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 :

: Carbon oxides

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products

Nitrogen oxides (NOx)

Hydrogen chloride gas

Specific extinguishing

methods

: No data available

Further information

: Remove container from danger zone and cool with

water.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures Advice for non-emergency personnel:

Avoid generation and inhalation of dusts in all

circumstances.

Avoid substance contact. Ensure adequate ventilation.

Keep away from heat and sources of ignition. 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

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Advice on protection against fire and explosion

: Keep away from open flames, hot surfaces and

sources of ignition.

Take precautionary measures against static discharge.

Advice on safe handling

: Work under hood. Do not inhale substance/mixture.

Further information on storage conditions

: Tightly closed.

Dry.

Keep in a well-ventilated place.

Keep locked up or in an area accessible only to

qualified or authorised persons.

Storage class : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very

toxic hazardous materials

Recommended storage

temperature

: 36 - 46 °F / 2 - 8 °C

Further information on

storage stability

: Moisture sensitive.

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 P3

The entrepeneur 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

Remarks : required

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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 : Flame retardant antistatic protective clothing.

Hygiene measures : Immediately change contaminated clothing. Apply

preventive skin protection. Wash hands and face

after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : Solidified mass or fragments

Color : colourless

to

light yellow

Odor : No data available

Odor Threshold : No data available pH : No data available

Melting point/ range : 79 - 84 °F / 26 - 29 °C

Method: lit.

Boiling point/boiling range : 397 - 399 °F / 203 - 204 °C

Method: lit.

Flash point : 194 °F / 90 °C

Method: closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Self-ignition : 1112 °F / 600 °C

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Upper explosion limit / Upper flammability limit

: No data available

Lower explosion limit / Lower flammability limit : No data available

Vapor pressure : 0.3 hPa (68 °F / 20 °C)

Relative vapour density : No data available

Relative density : No data available

Density : 1.2 g/mL (77 °F / 25 °C)

Method: lit.

Water solubility : No data available

Partition coefficient: n-

octanol/water

: log Pow: 3.12 (72 °F / 22 °C) Method: OECD Test Guideline 117 Bioaccumulation is not expected.

Autoignition temperature : 1112 °F / 600 °C

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 : 153.57 g/mol

Particle characteristics

Particle size : No data available

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

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distribution, when whirled up a dust explosion

potential may generally be assumed.

: The product is chemically stable under standard Chemical stability

ambient conditions (room temperature) .

Possibility of hazardous

reactions

: No data available

Conditions to avoid : Heat

Avoid moisture.

Strong heating.

Incompatible materials : Alcohols

> Strong bases Amines acids

Strong oxidizing agents

products

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

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 138 mg/kg

Remarks: (ECHA)

Acute toxicity estimate Inhalation - 4 h - 0.051 mg/l - dust/mist

(Expert judgement)

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h (OECD Test Guideline 404)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage.

(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Split adjuvant test - Guinea pig

Result: negative Remarks: (ECHA)

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May cause allergy or asthma symptoms or breathing difficulties if inhaled. Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal Method: OECD Test Guideline 474

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. - Lungs

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: NQ8575000

Cough, Shortness of breath, Headache, Nausea, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not

been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

4-Chloroisocyanatobenzene:

Toxicity to daphnia and : LC50 (Daphnia magna (Water flea)): 0.05 mg/l

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other aquatic End point: mortality invertebrates Exposure time: 48 h Analytical monitoring: yes

Analytical monitoring Remarks: (ECHA)

Ecotoxicology Assessment

Acute aquatic toxicity : Very toxic to aquatic life.

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

4-Chloroisocyanatobenzene:

Biodegradability : aerobic

Inoculum: activated sludge, non-adapted

Result: Not readily biodegradable.

Biodegradation: 0 % Exposure time: 20 d

Method: OECD Test Guideline 301D

Bioaccumulative potential

Components:

4-Chloroisocyanatobenzene:

Partition coefficient: n- : log Pow: 3.12 (72 °F / 22 °C) octanol/water : Method: OECD Test Guideline 117

Remarks: Bioaccumulation is not expected.

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).

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

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SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 2811

Proper shipping name : Toxic solid, organic, n.o.s.

(4-Chloroisocyanatobenzene)

Class : 6.1 Packing group : II

Labels : Division 6.1 - Toxic substances

Packing instruction (cargo: 676

aircraft)

Packing instruction : 669

(passenger aircraft)

IMDG-Code

UN number : UN 2811

Proper shipping name : TOXIC SOLID, ORGANIC, N.O.S.

(4-Chloroisocyanatobenzene)

Class : 6.1
Packing group : II
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2811

Proper shipping name : Toxic solids, organic, n.o.s.

(4-Chloroisocyanatobenzene)

Class : 6.1 Packing group : II

Labels : Division 6.1 - Toxic substances

ERG Code : 154 Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country 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 313 : The following components are subject to reporting

levels established by SARA Title III, Section 313:

4- 104-12-1 >= 90 - <= 100 %

Chloroisocyana tobenzene

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 SOCMI 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:

TSCA : All substances listed as active on the TSCA inventory

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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

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); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx -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; IC50 - 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; LC50 - Lethal Concentration to 50 % of a test population; LD50 - 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 quideline, 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 quarantee 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 Aldrich - 152277

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Revision Date : 09/19/2025

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