

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.13
Revision Date 04/27/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Phenyl isocyanate

Product Number : 78750
Brand : Sigma-Aldrich
CAS-No. : 103-71-9

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 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

Flammable liquids : Category 3

Acute toxicity (Oral)	: Category 4
Acute toxicity (Inhalation)	: Category 1
Skin corrosion	: Sub-category 1C
Serious eye damage	: Category 1
Respiratory sensitisation	: Category 1
Skin sensitisation	: Sub-category 1A
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	:	     
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Signal word	: Danger
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Hazard statements	: H226 Flammable liquid and vapour. H302 Harmful if swallowed. 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.
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Precautionary statements	: Prevention: P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P233 Keep container tightly closed. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof electrical/ ventilating/ lighting
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equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P260 Do not breathe mist or vapours.
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.

Response:

P301 + P330 + P331 + P310 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Immediately call a POISON CENTER/ doctor.
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.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance
Sigma-Aldrich - 78750

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CAS-No. : 103-71-9

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
phenyl isocyanate	103-71-9*	>= 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 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.
- 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 : Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : Foam
Water

Specific hazards during fire fighting : Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Nitrogen oxides (NO_x)

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:
Do not breathe vapours, 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.

Advice for emergency responders:
For personal protection see section 8.

- Environmental precautions : Do not let product enter drains.
Risk of explosion.
- 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- 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.
Avoid generation of vapours/aerosols.
- Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 3, Flammable liquids
- Recommended storage temperature : Recommended storage temperature see product label.
- Further information on storage stability : Moisture sensitive.
Store under inert gas.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
phenyl isocyanate	103-71-9	TWA	0.005 ppm	ACGIH
		STEL	0.015 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

Respiratory protection : 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.

Recommended Filter type: : Filter B-(P2)

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.

Hand protection

Material : Viton®
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material : butyl-rubber
Break through time : 30 min
Glove thickness : 0.7 mm
Protective index : Splash contact
Manufacturer : Butoject® (KCL 898)

Remarks : 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).

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	: liquid
Color	: No data available
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: -22 °F / -30 °C Method: lit.
Boiling point/boiling range	: 324 - 325 °F / 162 - 163 °C Method: lit.
Flash point	: 124 °F / 51 °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 998 hPa
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: 1.9 hPa (68 °F / 20 °C)
Relative vapour density	: No data available
Relative density	: 1.096 (67.3 °F / 19.6 °C)
Density	: 1.096 g/mL (77 °F / 25 °C) Method: lit.

Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: ca. 1193 °F / 645 °C Method: DIN 51794
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	: 119.12 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapour/air-mixtures are explosive at intense warming.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Exothermic reaction with: Amines alkalines Risk of ignition or formation of inflammable gases or vapours with: Alcohols Water Strong oxidizing agents Metals acids Risk of explosion with: nitrosyl compounds
Conditions to avoid	: Heat Avoid moisture. Heating.

Incompatible materials : No data available

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

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 887 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 0.022 mg/l - vapour

(OECD Test Guideline 403)

Inhalation: Corrosive to respiratory system.

LD50 Dermal - Rat - male - 5,000 mg/kg

Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 24 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. - 72 h

Remarks: (ECHA)

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

- Rat

Result: positive

Remarks: (ECHA)

Maximisation Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

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

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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

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: DA3675000

Cyanosis, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

phenyl isocyanate:

Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 10.6 mg/l
Exposure time: 96 h
Test Type: flow-through test
Analytical monitoring: yes
Remarks: (ECHA)

Toxicity to microorganisms : EC50 (Photobacterium phosphoreum): 20.21 mg/l
Exposure time: 30 min
Test Type: microtox test
Remarks: (IUCLID)

EC50 (activated sludge): 702 mg/l
Exposure time: 3 h
Method: OECD Test Guideline 209

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:

phenyl isocyanate:

Biodegradability : aerobic
Inoculum: activated sludge
Result: Readily biodegradable.
Biodegradation: 90 %
Exposure time: 30 d
Method: OECD Test Guideline 301D

Bioaccumulative potential

No data available

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).

Endocrine disrupting properties

No data available

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 waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not permitted for transport

IMDG-Code

UN number : UN 2487
Proper shipping name : PHENYL ISOCYANATE

Class : 6.1
Subsidiary risk : 3
Packing group : I
Labels : 6.1 (3)
EmS Code : F-E, S-D
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 2487
Proper shipping name : Phenyl isocyanate

Class : 6.1

Subsidiary risk : 3
Packing group : I
Labels : Division 6.1 - Poison inhalation hazard, Class 3 -
Flammable liquids

ERG Code : 155
Marine pollutant : no
Poison Inhalation Hazard : Hazard Zone B

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.

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 : Fire Hazard
Hazards Acute Health Hazard

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.

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 SOCM 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:

US 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

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
ACGIH / TWA : 8-hour, time-weighted average
ACGIH / STEL : Short-term exposure limit

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 -

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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 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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