

SAFETY DATA SHEET

Version 6.9
Revision Date 09/07/2024
Print Date 09/08/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Phenyl isocyanate

Product Number : 185353
Brand : 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

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)

Flammable liquids (Category 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 1), H330
Skin corrosion (Category 1C), H314

Serious eye damage (Category 1), H318
 Respiratory sensitization (Category 1), H334
 Skin sensitization (Sub-category 1A), 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

H226 Flammable liquid and vapor.
 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.

Precautionary Statements

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
 P233 Keep container tightly closed.
 P240 Ground/bond container and receiving equipment.
 P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
 P242 Use only non-sparking tools.
 P243 Take precautionary measures against static discharge.
 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

P333 + P313	rinsing. Immediately call a POISON CENTER/ doctor.
P342 + P311	If skin irritation or rash occurs: Get medical advice/ attention. If experiencing respiratory symptoms: Call a POISON CENTER/ doctor.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391	Collect spillage.
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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	: C ₇ H ₅ NO
Molecular weight	: 119.12 g/mol
CAS-No.	: 103-71-9
EC-No.	: 203-137-6

Component	Classification	Concentration
phenyl isocyanate		
	Flam. Liq. 3; Acute Tox. 4; Acute Tox. 1; Skin Corr. 1C; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1A; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H226, H302, H330, 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)

Combustible.

Vapors 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.

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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. Risk of explosion.

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.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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

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 authorized persons.

Storage stability

 Recommended storage temperature

2 - 8 °C

Store under inert gas. Moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

Component	CAS-No.	Value	Control parameters	Basis
phenyl isocyanate	103-71-9	TWA	0.005 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Dermal Sensitization Respiratory sensitization Danger of cutaneous absorption		
		STEL	0.015 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Dermal Sensitization Respiratory sensitization Danger of cutaneous absorption		

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: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 30 min

Material tested: Butoject® (KCL 898)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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.

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: -30 °C (-22 °F) - lit.
f) Initial boiling point and boiling range	162 - 163 °C 324 - 325 °F - lit.
g) Flash point	51 °C (124 °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) Vapor pressure	1.9 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	1.096 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	1.09619.6 °C
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	> 600 °C (> 1112 °F) at 998 hPa

- 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

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 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

10.4 Conditions to avoid

Heat. Avoid moisture.

Heating.

10.5 Incompatible materials

No data available

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

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 - vapor

(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)

Maximization 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 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. - 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**12.1 Toxicity**

Toxicity to fish flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 10.6 mg/l - 96 h
Remarks: (ECHA)

Toxicity to bacteria Remarks: (IUCLID)
(phenyl isocyanate)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 30 d
Result: 90 % - 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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

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: 2487 Class: 6.1I (3) Packing group: I

Proper shipping name: Phenyl isocyanate

Reportable Quantity (RQ):

Poison Inhalation Hazard: Hazard Zone B

IMDG

UN number: 2487 Class: 6.1 (3) Packing group: I

EMS-No: F-E, S-D

Proper shipping name: PHENYL ISOCYANATE

IATA

UN number: 2487 Class: 6.1 (3)

Proper shipping name: Phenyl isocyanate

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

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 Hazards : Fire Hazard
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.

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 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.9

Revision Date: 09/07/2024

Print Date: 09/08/2024