

## SAFETY DATA SHEET

Version 6.6  
Revision Date 09/12/2021  
Print Date 05/28/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 1,4-Phenylene diisocyanate

Product Number : 262242  
Brand : Aldrich  
CAS-No. : 104-49-4

**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, Inhalation (Category 2), H330  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Respiratory sensitization (Category 1), H334  
Skin sensitization (Category 1), H317  
Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (Category 2), H411

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)	
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
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/ eye protection/ face protection.
P284	Wear respiratory protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and 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	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333 + P313	If skin irritation or rash 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.
P391	Collect spillage.
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>4</sub> N <sub>2</sub> O <sub>2</sub>
Molecular weight	: 160.13 g/mol
CAS-No.	: 104-49-4
EC-No.	: 203-207-6

Component	Classification	Concentration
<b>p-Phenylene diisocyanate</b>		
	Acute Tox. 2; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; Aquatic Acute 2; Aquatic Chronic	<= 100 %

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	2; H330, H315, H319, H334, H317, H401, H411	
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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

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. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

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.

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## SECTION 6: Accidental release measures

### 6.1 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. 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. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 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

Work under hood. Do not inhale substance/mixture.

#### 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. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Air and 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

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). Safety glasses

#### Skin protection

Handle with impervious gloves.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

#### Body Protection

protective clothing

#### 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.

### 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: crystalline<br>Color: white, to, yellow         |
| b) Odor                         | No data available                                     |
| c) Odor Threshold               | No data available                                     |
| d) pH                           | No data available                                     |
| e) Melting point/freezing point | Melting point/range: 96 - 99 °C (205 - 210 °F) - lit. |
| f) Initial boiling point        | 260 °C 500 °F - lit.                                  |

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and boiling range

- |   |                                  |
|---|----------------------------------|
| g) Flash point                                  | > 113 °C (> 235 °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                               | < 0.01 hPa at 20 °C (68 °F)      |
| l) Vapor density                                | No data available                |
| m) Density                                      | No data available                |
| Relative density                                | No data available                |
| n) Water solubility                             | ca.130 g/l at 20 °C (68 °F)      |
| 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

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## 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.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Air

Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents, Amines, Strong bases, Strong acids

## 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

LD50 Oral - Rat - female - 5,000 mg/kg

(OECD Test Guideline 423)

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

(Expert judgment)

Acute toxicity estimate Inhalation - Expert judgment - 4 h - 0.051 mg/l

Dermal: No data available

#### Skin corrosion/irritation

Causes skin irritation.

#### Serious eye damage/eye irritation

Causes serious eye irritation.

#### Respiratory or skin sensitization

May cause allergic respiratory and skin reactions

#### Germ cell mutagenicity

No data available

#### 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

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

### 11.2 Additional Information

RTECS: CZ6150000

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	static test LC50 - Oncorhynchus mykiss (rainbow trout) - 133 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 4.46 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 25.46 mg/l - 48 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - activated sludge - $\geq 1,000$ mg/l - 3 h (OECD Test Guideline 209)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 10.46 % - Not readily biodegradable. (OECD Test Guideline 301B)
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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 Other adverse effects

No data available

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## 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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2811    Class: 6.1    Packing group: II  
Proper shipping name: Toxic solids, organic, n.o.s. (p-Phenylene diisocyanate)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

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UN number: 2811 Class: 6.1 Packing group: II EMS-No: F-A, S-A  
Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (p-Phenylene diisocyanate)  
Marine pollutant : yes

**IATA**

UN number: 2811 Class: 6.1 Packing group: II  
Proper shipping name: Toxic solid, organic, n.o.s. (p-Phenylene diisocyanate)

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**SECTION 15: Regulatory information**

**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

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**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**

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**New Jersey Right To Know Components**

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**SECTION 16: Other information**

**Further information**

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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