

Chemical Safety Data Sheet MSDS / SDS

1,4-Phenylene diisocyanate

Revision Date:2026-06-06 Revision Number:1

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

Product name : 1,4-Phenylene diisocyanate
CBnumber : CB5409756
CAS : 104-49-4
EINECS Number : 203-207-6
Synonyms : PPDI,1,4-Phenylene diisocyanate

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H330 Fatal if inhaled

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H315 Causes skin irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1,4-Phenylene diisocyanate
Synonyms	: PPDI, 1,4-Phenylene diisocyanate
CAS	: 104-49-4
EC number	: 203-207-6
MF	: C ₈ H ₄ N ₂ O ₂
MW	: 160.13

SECTION 4: 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.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 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. 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.

Hazardous combustion products

Carbon oxides Nitrogen oxides (NOx)

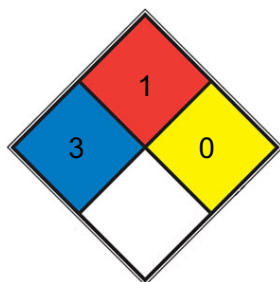
Specific extinguishing methods

Suppress (knock down) gases/vapors/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.

NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

□ SPEC.
□ HAZ.

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. 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

Handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Avoidance of contact

Strong oxidizing agents Amines Strong bases Strong acids

Storage

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 authorized persons.

Storage class

6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

Recommended storage temperature

Recommended storage temperature see product label.

Further information on storage stability

Air and moisture sensitive. Handle and store under inert gas.

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 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.

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 and body protection

protective clothing

Hand protection**Material**

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Full contact

Manufacturer

KCL 741 L

Material

Nitrile rubber

Break through time

480 min

Glove thickness

0.11 mm

Protective index

Splash contact

Manufacturer

KCL 741 L

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).

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

crystalline

Color

white, to, yellow

Odor

No data available

Odor Threshold

No data available

pH

No data available

pH

7

Melting point/ range

96 - 99 °C

Method: lit.

Boiling point/boiling range

260 °C

Method: lit.

Flash point

> 113 °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

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

< 0.01 hPa (20 °C)

Relative vapor density

No data available

Relative density

1.3848 (rough estimate)

Density

1.3848 (rough estimate)

Water solubility

ca. 130 g/l (20 °C)

Partition coefficient: n-octanol/water

No data available

Autoignition temperature

No data available

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

160.13 g/mol

Particle characteristics Particle size

No data available

Solubility

THF: soluble

Physical state

powder to crystal

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 distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

Air Strong heating.

Incompatible materials

Strong oxidizing agents Amines Strong bases Strong acids

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 - female - 5,000 mg/kg (OECD Test Guideline 423)

Acute toxicity estimate Inhalation - 4 h - 0.051 mg/l - dust/mist (Expert judgment)

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

LD50 Dermal - female - \geq 2,000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Remarks: Causes skin irritation.

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.

Respiratory or skin sensitization

May cause allergic respiratory and skin reactions

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

RTECS: CZ6150000

SECTION 12: Ecological information

Ecotoxicity

Components:

p-Phenylene diisocyanate:

Toxicity to fish

LC50 (Oncorhynchus mykiss (rainbow trout)): 133 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

EC50 (Daphnia magna (Water flea)): 4.46 mg/l End point: mortality Exposure time: 48 h Test Type: static test Method: OECD Test Guideline 202 GLP: yes

Toxicity to algae/aquatic plants

ErC50 (Pseudokirchneriella subcapitata): 25.46 mg/l Exposure time: 48 h Test Type: static test Method: OECD Test Guideline 201 GLP: yes

Toxicity to microorganisms

EC50 (activated sludge): \geq 1,000 mg/l Exposure time: 3 h Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

p-Phenylene diisocyanate:

Biodegradability

aerobic Inoculum: activated sludge, adapted Concentration: 0.25 mg/l Result: Not readily biodegradable. Biodegradation: 10.46 % Exposure time: 28 d Method: OECD Test Guideline 301B GLP: yes

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 2811

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

(p-Phenylene diisocyanate)

Class : 6.1

Packing group : II

Labels : Division 6.1 - Toxic substances

Packing instruction (cargo aircraft) : 676

Packing instruction (passenger aircraft) : 669

IMDG-Code

UN number : UN 2811

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

(p-Phenylene diisocyanate)

Class : 6.1

Packing group : II

Labels : 6.1

EmS Code : F-A, S-A

Marine pollutant : yes

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : UN 2811

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

(p-Phenylene diisocyanate)

Class : 6.1

Packing group : II

Labels : 6.1

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

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Listed

No. / Code Chemical name / Category Threshold quantity

J5 Acute toxic 500 t

Hazardous Chemicals for Priority Management

Listed under SAWS

Regulations on Occupational Labor Protection in the at workplaces where

Toxic Substances Are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

SECTION 16: Other information

Full text of other abbreviations

AllC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight
 CMR - Carcinogen, Mutagen or Reproductive Toxicant
 DIN -Standard of the German Institute for Standardisation
 DSL - Domestic SubstancesList (Canada)
 ECx - Concentration associated with x% response
 ELx - Loading rate associated with x% response
 EmS - Emergency Schedule
 ENCS - Existing and NewChemical Substances (Japan)
 ErCx - Concentration associated with x% growth rate response
 ERG - Emergency Response Guide
 GHS - Globally Harmonized System
 GLP - Good Laboratory Practice
 IARC - International Agency for Research on Can- cer
 IATA - International Air Transport Association
 IBC - International Code for theConstruction and Equipment of Ships carrying Dangerous Chemicals in Bulk
 IC50 -Half maximal inhibitory concentration
 ICAO - International Civil Aviation Organiza- tion
 IECSC - Inventory of Existing Chemical Substances in China
 IMDG - Interna- tional Maritime Dangerous Goods
 IMO - International Maritime Organization
 ISHL -Industrial Safety and Health Law (Japan)
 ISO - International Organisation forStandardization
 KECI - Korea Existing Chemicals Inventory
 LC50 - Lethal Concen- tration 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 Pol- lution from Ships
 n.o.s. - Not Otherwise Specified
 Nch - Chilean Norm
 NO(A)EC -No Observed (Adverse) Effect Concentration
 NO(A)EL - No Observed (Adverse) Ef- fect Level
 NOELR - No Observable Effect Loading Rate
 NOM - Official MexicanNorm
 NTP - National Toxicology Program
 NZIoC - New Zealand Inventory of Chem- icals
 OECD - Organization for Economic Co-operation and Development
 OPPTS - Of- fice of Chemical Safety and Pollution Prevention
 PBT - Persistent, Bioaccumulative and Toxic substance
 PICCS - Philippines Inventory of Chemicals and Chemical Sub- stances
 (Q)SAR - (Quantitative) Structure Activity Relationship
 REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning theRegistration, Evaluation, Authorisation and Restriction of Chemicals
 SADT - Self-Accelerating Decomposition Temperature
 SDS - Safety Data Sheet
 TCSI - TaiwanChemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI -Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (UnitedStates)

UN - United Nations

UNRTDG - United Nations Recommendations on theTransport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.