

## Chemical Safety Data Sheet MSDS / SDS

**1,4-PHENYLENE DIISOTHIOCYANATE**

Revision Date:2024-12-21 Revision Number:1

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

Product name : 1,4-PHENYLENE DIISOTHIOCYANATE  
CBnumber : CB5292882  
CAS : 4044-65-9  
EINECS Number : 223-741-3  
Synonyms : pditc, 1,4-diisothiocyanatobenzene

**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 : 400-158-6606

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

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P501 Dispose of contents/container to.....

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P391 Collect spillage. Hazardous to the aquatic environment

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

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

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P284 Wear respiratory protection.

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

P273 Avoid release to the environment.

P271 Use only outdoors or in a well-ventilated area.

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

#### **Hazard statements**

H410 Very toxic to aquatic life with long lasting effects

H400 Very toxic to aquatic life

H335 May cause respiratory irritation

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

H331 Toxic if inhaled

H319 Causes serious eye irritation

H318 Causes serious eye damage

H315 Causes skin irritation

H314 Causes severe skin burns and eye damage

H312 Harmful in contact with skin

H302 Harmful if swallowed

H301 Toxic if swallowed

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 1,4-PHENYLENE DIISOTHIOCYANATE
Synonyms	: pditc, 1,4-diisothiocyanatobenzene
CAS	: 4044-65-9
EC number	: 223-741-3
MF	: C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub>
MW	: 192.26

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### **In case of skin contact**

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### **In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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 2.2) and/or in section 11

#### Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides Combustible.

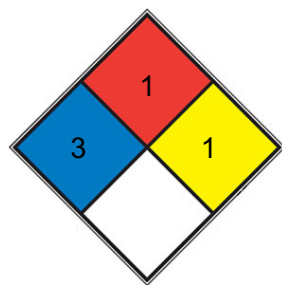
#### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### Further information

No data available

#### 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 1** Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

**SPEC.**

**HAZ.**

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## SECTION 6: Accidental release measures

## **Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

## **Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## **Methods and materials for containment and cleaning up**

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

## **Reference to other sections**

For disposal see section 13.

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# **SECTION 7: Handling and storage**

## **Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

## **Conditions for safe storage, including any incompatibilities**

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Moisture sensitive. Store under inert gas.

## **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**

## **control parameter**

### **Hazard composition and occupational exposure limits**

Does not contain substances with occupational exposure limits.

## **Exposure controls**

### **Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### **Personal protective equipment**

#### **Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### **Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory

practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatrill? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	beige powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 129 - 131 °C - lit.
Initial boiling point and boiling range	339.4±25.0 °C(Predicted)
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	chloroform: clear
Partition coefficient: n-octanol/water	No data available

Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

No data available

### Incompatible materials

Strong oxidizing agents, Strong acids, Strong bases

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Sulphur oxides

Other decomposition products - No data available In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Mouse - 230 mg/kg

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation Germ cell mutagenicity

No data available

#### 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.

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.

#### **Reproductive toxicity**

No data available

#### **Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

#### **Additional Information**

RTECS: NX9150000

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

#### **Toxicity**

LD50 oral in mouse: 230mg/kg

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## SECTION 12: Ecological information

### **Toxicity**

#### **Toxicity to daphnia and other aquatic invertebrates**

LC50 - Daphnia magna (Water flea) - 0,077 mg/l - 48 h

#### **Persistence and degradability**

No data available

#### **Bioaccumulative potential**

No data available

#### **Mobility in soil**

No data available

#### **Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### **Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### **Waste treatment methods**

## Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

### Incompatibilities

Incompatible with oxidizers (chlorates, nitrates, peroxides, permanganates, perchlorates, chlorine, bromine, fluorine, etc.); contact may cause fires or explosions. Keep away from alkaline materials, strong bases, strong acids, oxoacids, epoxides.

### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### UN number

ADR/RID: 2811 IMDG: 2811 IATA: 2811

### UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (Bitoscanate) IMDG: TOXIC SOLID, ORGANIC, N.O.S. (Bitoscanate)

IATA: Toxic solid, organic, n.o.s.  
(Bitoscanate)

14.3	Transport hazard class(es) ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group ADR/RID: III IMDG: III	IATA: III
14.5	Environmental hazards ADR/RID: no IMDG Marine pollutant: no	IATA: no
14.6	Special precautions for user No data available	

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## SECTION 15: Regulatory information

### Safety, health and environmental regulations/legislation specific for the substance or mixture

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>



Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Not Listed. website: <https://www.mee.gov.cn/>

Korea Existing Chemicals List (KECL): Not Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Not Listed. website: <https://emb.gov.ph/>

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## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

### References

【1】CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

#### 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.