

## Chemical Safety Data Sheet MSDS / SDS

## Phthalonitrile

Revision Date:2025-02-01 Revision Number:1

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

## Product identifier

Product name : Phthalonitrile  
CBnumber : CB2773751  
CAS : 91-15-6  
EINECS Number : 202-044-8  
Synonyms : phthalonitrile, 1,2-Benzenedicarbonitrile

## 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

P405 Store locked up.  
P321 Specific treatment (see ... on this label).  
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.

## Hazard statements

H311 Toxic in contact with skin  
H300 Fatal if swallowed

## SECTION 3: Composition/information on ingredients

## Substance

Product name	: Phthalonitrile
Synonyms	: phthalonitrile, 1,2-Benzenedicarbonitrile
CAS	: 91-15-6
EC number	: 202-044-8
MF	: C <sub>8</sub> H <sub>4</sub> N <sub>2</sub>
MW	: 128.13

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this material 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

Flush eyes with water as a precaution.

#### 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>)

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

No data available

## NFPA 704



☒ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

☒ FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

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

☐ 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 vapors, 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.

### **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:Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

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

Material tested:Dermatril? (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 EC 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 N100 (US) or type P3 (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 crystalline
Odour	No data available
Odour Threshold	No data available
pH	7 (H <sub>2</sub> O)
Melting point/freezing point	Melting point/range: 137 - 139 °C - lit.
Initial boiling point and boiling range	227.54°C (rough estimate)
Flash point	162 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	<1 Pa (25 °C)
Vapour density	No data available
Relative density	No data available
Water solubility	benzene: 50 mg/mL, 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 acids, Strong bases, Strong oxidizing agents, Strong reducing agents

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

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 - Rat - male and female - 125 mg/kg (OECD Test Guideline 401)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 20 h Remarks: (ECHA)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation (OECD Test Guideline 405)

#### **Respiratory or skin sensitization**

(OECD Test Guideline 429)

#### **Germ cell mutagenicity**

Ames test

Salmonella typhimurium Result: negative

OECD Test Guideline 474 Mouse - male and female 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.

#### **Reproductive toxicity**

**Specific target organ toxicity - single exposure Specific target organ toxicity - repeated exposure Aspiration hazard**

#### **Additional Information**

RTECS: Not available

Systemic effects:

After absorption:

Convulsions, Unconsciousness Symptoms may be delayed.

Other information

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

#### **Toxicity**

## SECTION 12: Ecological information

### Toxicity

#### Toxicity to fish

semi-static test LC50 - *Oryzias latipes* (Orange-red killifish) - 22,6 mg/l - 96 h

(OECD Test Guideline 203)

#### Toxicity to daphnia and other aquatic invertebrates

static test EC50 - *Daphnia magna* (Water flea) - 219 mg/l - 48 h (US-EPA)

#### Toxicity to algae

static test ErC50 - *Pseudokirchneriella subcapitata* (green algae) - 140 mg/l - 72 h

(OECD Test Guideline 201)

### Persistence and degradability

Biodegradability aerobic Dissolved organic carbon (DOC) - Exposure time 28 d Result: 55 % - Not readily biodegradable.

(OECD Test Guideline 301E)

Biochemical Oxygen Demand (BOD)

Chemical Oxygen Demand (COD)

< 10 mg/g

Remarks: (External MSDS)

1.015 mg/g

Remarks: (External MSDS)

### Bioaccumulative potential

Bioaccumulation *Cyprinus carpio* (Carp) - 42 d

- 0,2 mg/l(phthalonitrile)

Bioconcentration factor (BCF): < 5,5 (OECD Test Guideline 305C)

### Mobility in soil

### 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

Additional ecological information

Biological effects:

When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected. Further information on ecology

Discharge into the environment must be avoided.

## 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.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### UN number

ADR/RID: 3439 IMDG: 3439 IATA: 3439

### UN proper shipping name

ADR/RID: NITRILES, SOLID, TOXIC, N.O.S. (phthalonitrile) IMDG: NITRILES, SOLID, TOXIC, N.O.S. (phthalonitrile)

IATA: Nitriles, solid, toxic, n.o.s.  
(phthalonitrile)

14.3	Transport hazard class(es) ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group ADR/RID: II IMDG: II	IATA: II
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

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

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

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>



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

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

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

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

EC Inventory:Listed.

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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.