

## Chemical Safety Data Sheet MSDS / SDS

**4-Nitro-1,3-phenylenediamine**

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

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

Product name : 4-Nitro-1,3-phenylenediamine  
CBnumber : CB9434172  
CAS : 5131-58-8  
EINECS Number : 225-876-3  
Synonyms : 4-nitrobenzene-1,3-diamine,4-Nitro-1,3-phenylenediamine

**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****Classification of the substance or mixture**

Acute toxicity - Category 4, Oral  
Skin irritation, Category 2  
Skin sensitization, Category 1

**Label elements****Pictogram(s)**

☐☐

Signal word : Warning

**Hazard statement(s)**

H301 Toxic if swallowed  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H341 Suspected of causing genetic defects

**Precautionary statement(s)**

P201 Obtain special instructions before use.

P264 Wash hands thoroughly after handling.

P264 Wash skin thoroughly after handling.

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

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

Continuerinsing.

P405 Store locked up.

#### **Prevention**

P264 Wash ... thoroughly after handling.

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

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

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

P272 Contaminated work clothing should not be allowed out of the workplace.

#### **Response**

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P333+P317 If skin irritation or rash occurs: Get medical help.

#### **Storage**

none

#### **Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

#### **Other hazards**

no data available

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 4-Nitro-1,3-phenylenediamine
Synonyms	: 4-nitrobenzene-1,3-diamine,4-Nitro-1,3-phenylenediamine
CAS	: 5131-58-8
EC number	: 225-876-3
MF	: C6H7N3O2
MW	: 153.14

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## SECTION 4: First aid measures

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

**If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

**Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

**Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

**Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

**Most important symptoms and effects, both acute and delayed**

no data available

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

no data available

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## SECTION 5: Firefighting measures

**Extinguishing media**

Fires involving this compound can be controlled using a carbon dioxide, dry chemical or Halon extinguisher. (NTP, 1992)

**Specific Hazards Arising from the Chemical**

Flash point data for this chemical are not available, but it is probably combustible. (NTP, 1992)

**Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**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**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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## SECTION 7: Handling and storage

### **Precautions for safe handling**

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### **Control parameters**

#### **Occupational Exposure limit values**

no data available

#### **Biological limit values**

no data available

### **Exposure controls**

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### **Individual protection measures**

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

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	Solid. Solid.
Colour	Yellow compound in hair dyes
Odour	no data available
Melting point/freezing point	161 °C. Remarks:Other details not available.
Boiling point or initial boiling point and boiling range	326.23 °C. Remarks:Estimated value.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	160.79 °C. Atm. press.:1 atm.pres.
Auto-ignition temperature	> 500 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 1 mg/mL at 68.9° F (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = 0.55. Remarks:Estimated data.
Vapour pressure	0.007 Pa. Temperature:25 °C. Remarks:Estimated data.
Density and/or relative density	1.552 g/cm <sup>3</sup> . Temperature:19.85 °C.
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

4-NITRO-1,3-BENZENEDIAMINE is an amine/organonitrate. Amines are chemical bases. They neutralize acids to form salts plus water. These

acid-base reactions are exothermic. The amount of heat that is evolved per mole of amine in a neutralization is largely independent of the strength of the amine as a base. Amines may be incompatible with isocyanates, halogenated organics, peroxides, phenols (acidic), epoxides, anhydrides, and acid halides. Flammable gaseous hydrogen is generated by amines in combination with strong reducing agents, such as hydrides.

#### **Conditions to avoid**

no data available

#### **Incompatible materials**

no data available

#### **Hazardous decomposition products**

no data available

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## SECTION 11: Toxicological information

#### **Acute toxicity**

- Oral: LD50 Mouse oral 500 mg/kg
- Inhalation: no data available
- Dermal: no data available

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

no data available

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

no data available

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

no data available

#### **Germ cell mutagenicity**

no data available

#### **Carcinogenicity**

no data available

#### **Reproductive toxicity**

no data available

#### **STOT-single exposure**

no data available

#### **STOT-repeated exposure**

no data available

## Aspiration hazard

no data available

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## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 101.8 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 221 mg/L - 48 h.

Toxicity to algae: EC50 - green algae - 160 mg/L - 72 h.

Toxicity to microorganisms: no data available

### Persistence and degradability

no data available

### Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for 4-nitro-1,3-benzenediamine(SRC), using an estimated log Kow of 0.55(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

### Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 4-nitro-1,3-benzenediamine can be estimated to be 85(SRC). According to a classification scheme(2), this estimated Koc value suggests that 4-nitro-1,3-benzenediamine is expected to have high mobility in soil(SRC). However, aromatic amines are expected to bind strongly to humus or organic matter in soils due to the high reactivity of the aromatic amino group(3), suggesting that mobility may be much lower in some soils(SRC).

### Other adverse effects

no data available

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## SECTION 13: Disposal considerations

### Disposal methods

#### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

### **Special precautions for user**

no data available

### **Transport in bulk according to IMO instruments**

no data available

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## SECTION 15: Regulatory information

### **Safety, health and environmental regulations specific for the product in question**

#### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

#### **EC Inventory**

Listed.

#### **United States Toxic Substances Control Act (TSCA) Inventory**

Listed.

#### **China Catalog of Hazardous chemicals 2015**

Not Listed.

#### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.



**PICCS**

Listed.

**Vietnam National Chemical Inventory**

Not Listed.

**IECSC**

Listed.

**Korea Existing Chemicals List (KECL)**

Listed.

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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

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

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### References

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

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

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

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)

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

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

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

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

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

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