

## Chemical Safety Data Sheet MSDS / SDS

## 4-nitroaniline SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 4-nitroaniline  
CAS: 100-01-6

**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.in  
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090  
Telephone: +91 9550333722

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Acute toxicity - Category 3, Oral  
Acute toxicity - Category 3, Dermal

Acute toxicity - Category 3, Inhalation  
Specific target organ toxicity - repeated exposure, Category 2  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

### GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

### Hazard statement(s)

H301 Toxic if swallowed  
H311 Toxic in contact with skin  
H331 Toxic if inhaled  
H373 May cause damage to organs through prolonged or repeated exposure  
H412 Harmful to aquatic life with long lasting effects

### Precautionary statement(s)

### 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.  
P271 Use only outdoors or in a well-ventilated area.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P273 Avoid release to the environment.

### Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.  
P321 Specific treatment (see ... on this label).  
P330 Rinse mouth.  
P302+P352 IF ON SKIN: Wash with plenty of water/...  
P316 Get emergency medical help immediately.  
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P319 Get medical help if you feel unwell.

### Storage

P405 Store locked up.

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

### 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 which do not result in classification

no data available

## SECTION 3: Composition/information on ingredients

### Substance

Chemical name: 4-nitroaniline

Common names and synonyms: 4-nitroaniline

CAS number: 100-01-6

EC number: 202-810-1

Concentration: 100%

## SECTION 4: First aid measures

### Description of necessary first-aid measures

#### If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

#### Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

#### Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

### **Following ingestion**

Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention .

### **Most important symptoms/effects, acute and delayed**

Inhalation or ingestion causes headache, drowsiness, shortness of breath, nausea, methemoglobinemia, and unconsciousness; fingernails, lips, and ears become bluish; prolonged and excessive exposures may also cause liver damage. Contact with eyes causes irritation and possible corneal damage. Contact with skin causes irritation; continued exposure may cause same symptoms as inhalation or ingestion. (USCG, 1999)

### **Indication of immediate medical attention and special treatment needed, if necessary**

INHALATION: Fresh air, rest. Artificial respiration if indicated. Refer for medical attention. SKIN: Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention. EYES: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then take to a doctor.

## **SECTION 5: Firefighting measures**

### **Suitable extinguishing media**

This chemical is a combustible solid. Use dry chemical, carbon dioxide, water spray, or alcohol foam extinguishers. Poisonous gases including sulfur dioxide and nitrogen oxides are produced in fire. If material or contaminated runoff enters waterways, notify downstream users of potentially contaminated waters. Notify local health and fire officials and pollution control agencies. From a secure, explosion-proof location, use water spray to cool exposed containers. If cooling streams are ineffective (venting sound increases in volume and pitch, tank discolors, or shows any signs of deforming), withdraw immediately to a secure position. If employees are expected to fight fires, they must be trained and equipped in OSHA 1910.156.

### **Specific hazards arising from the chemical**

Special Hazards of Combustion Products: Toxic oxides of nitrogen may form in fire. Behavior in Fire: Melts and burns (USCG, 1999)

### **Special protective actions for fire-fighters**

Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water. Combat fire from a sheltered position.

## **SECTION 6: Accidental release measures**

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

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

### **Environmental precautions**

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Wash away remainder with plenty of water.

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

1. Ventilate area of spill. 2. For small quantities, sweep onto paper or other suitable material, place in an appropriate container & burn in a safe place (such as a fume hood). Large quantities may be reclaimed; however, if this is not practical, dissolve in a flammable solvent (such as alcohol) & atomize in a suitable combustion chamber equipped with an appropriate effluent gas cleaning device.

## **SECTION 7: Handling and storage**

### **Precautions for safe handling**

NO open flames. NO contact with combustible substances. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. 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**

Separated from strong acids, strong oxidants, combustible substances, reducing agents and food and feedstuffs. Dry. Store in a cool, dry, well-ventilated location. Separate from acids, oxidizing materials, & reducing agents.

## **SECTION 8: Exposure controls/personal protection**

### **Control parameters**

### **Occupational Exposure limit values**

TLV: 3 mg/m<sup>3</sup>, as TWA; (skin); A4 (not classifiable as a human carcinogen); BEI issued. MAK: skin absorption (H); carcinogen category: 3A

### Biological limit values

no data available

### Appropriate engineering 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, such as personal protective equipment (PPE)

#### Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

#### Skin protection

Protective gloves. Protective clothing.

#### Respiratory protection

Use local exhaust or breathing protection.

#### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Powder.
Colour:	Brown.
Odour:	Faint ammonia; slightly pungent
Melting point/freezing point:	158 °C. Atm. press.:975 hPa. Remarks:Other details not available.
Boiling point or initial boiling point and boiling range:	> 800 °C. Atm. press.:975 hPa. Remarks:Other details not available.
Flammability:	Combustible Solid

Lower and upper explosion limit/flammability limit:	no data available
Flash point:	100.8 °C. Atm. press.:975 hPa.
Auto-ignition temperature:	Atm. press.:975 hPa. Remarks:4-nitroaniline did not catch fire on being exposed to air at room temperature of 30 degC.
Decomposition temperature:	no data available
pH:	7.45. Remarks:Neutral.
Kinematic viscosity:	no data available
Solubility:	Insoluble in water
Partition coefficient n-octanol/water:	log Pow = 1.2. Temperature:30 °C.
Vapour pressure:	3 Pa. Temperature:100 °C. Remarks:At 20 oC, 3 Pascal is equivalent to 0.6 Pa.
Density and/or relative density:	0.951 g/cm <sup>3</sup> . Temperature:30 °C.
Relative vapour density:	4.77 (NTP, 1992) (Relative to Air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

May explode on heating. On combustion, forms toxic fumes of nitrogen oxides. Reacts with strong acids, strong oxidants and strong reducing agents. Reacts with organic materials in the presence of moisture. This generates fire hazard.

### Chemical stability

no data available

### **Possibility of hazardous reactions**

Combustible when exposed to heat or flame. Dust explosion possible if in powder or granular form, mixed with air. P-NITROANILINE may react vigorously with sulfuric acid above 392° F. It may also react with sodium hydroxide at 266° F. Under pressure, it may produce an explosive compound. It is incompatible with strong oxidizers and strong reducing agents. It is capable of explosive decomposition with strong initiators. It will attack some forms of plastics, rubber and coatings. (NTP, 1992)

### **Conditions to avoid**

no data available

### **Incompatible materials**

An ammoniacal soln of 4-nitroaniline containing ammonium chloride was being treated with 50% sodium hydroxide soln to displace ammonia. In error, double the amt required to give usual 10% of free alkali was added, & during subsequent degassing operation (heating to 130 deg C under pressure, followed by depressuring to vent ammonia), complete conversion to sodium 4-nitrophenoxide occurred. ... /When/ separated by centrifuging, it was then heated to dry ... when it decomposed violently & was ejected through the vessel opening. ... Some of the tautomeric aci-nitroquinonoid salt may have been produced during the drying operation.

### **Hazardous decomposition products**

Explosive decomposition may occur under fire conditions.

## **SECTION 11: Toxicological information**

### **Acute toxicity**

Oral: LD50 - Bird - wild bird species - 75 mg/kg bw.

Inhalation: LC50 - rat (male) - 47.485 ppm.

Dermal: LD50 - guinea pig - > 500 mg/kg bw.

### **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**

A4; Not classifiable as a human carcinogen.

#### **Reproductive toxicity**

no data available

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

The substance is mildly irritating to the eyes. The substance may cause effects on the blood. This may result in the formation of methaemoglobin. The effects may be delayed. Medical observation is indicated. See Notes.

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

The substance may have effects on the blood. This may result in the formation of methaemoglobin. See Notes.

#### **Aspiration hazard**

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C , on spraying or dispersing much faster.

## **SECTION 12: Ecological information**

#### **Toxicity**

Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - 87.6 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - Daphnia magna - 24 mg/L - 24 h.

Toxicity to algae: EC50 - Chlorococcales - 68 mg/L - 24 h.

Toxicity to microorganisms: IC50 - Tetrahymena pyriformis - 10.14 mg/L - 60 h.

#### **Persistence and degradability**

P-nitroaniline at concn 250-1000 mg/l was degraded by a mixt of pseudomonas fluorescens & bacillus valinovorius.

#### **Bioaccumulative potential**

In a 6-week bioconcentration test, the BCF of 4-nitroaniline was 2.9-3.6 at a concentration of 0.5 mg/L and <10 at a concentration of 0.05 mg/L(1). In a bioconcentration study using zebrafish and a 4-nitroaniline concentration of 0.21 umol/L, the BCF was measured to be 4.4(2). According to a classification scheme(3), these experimental BCF values suggest bioconcentration in aquatic organisms is low (SRC).

#### **Mobility in soil**

4-Nitroaniline has measured log Koc values of 1.78(1) and 1.88(2) and log Kom values of 1.49(3) and 1.64(4). These values correspond to Koc values of 60, 76, 54 and 75, respectively. 4-Nitroaniline has also been observed to have a Koc of 87(5). According to a classification scheme(6), these Koc values suggest that 4-nitroaniline is expected to have high mobility in soil. 4-Nitroaniline was found to have a Kd value of 13.5 L/kg in homoionic K+ Montmorillonite type soil(7). However, anilines are expected to bind strongly to humus or organic matter in soils due to the high reactivity of the aromatic amino group(8,9), suggesting that mobility may be much lower in some soils(SRC). 4-Nitroaniline had small and scattered amounts of irreversible binding over a 20 hour experiment(10).

#### **Other adverse effects**

no data available

### **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.

## SECTION 14: Transport information

### UN Number

ADR/RID: UN1661 (For reference only, please check.)

IMDG: UN1661 (For reference only, please check.)

IATA: UN1661 (For reference only, please check.)

### UN Proper Shipping Name

ADR/RID: NITROANILINES (o-, m-, p-) (For reference only, please check.)

IMDG: NITROANILINES (o-, m-, p-) (For reference only, please check.)

IATA: NITROANILINES (o-, m-, p-) (For reference only, please check.)

### Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

### Packing group, if applicable

ADR/RID: II (For reference only, please check.)

IMDG: II (For reference only, please check.)

IATA: II (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

### **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**

Listed.

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

Listed.

**(PICCS)**

Listed.

**Vietnam National Chemical Inventory**

Listed.

**IECSC)**

Listed.

**Korea Existing Chemicals List (KECL)**

Listed.

### **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/>

### **Other Information**

Depending on the degree of exposure, periodic medical examination is indicated. Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available. See ICSCs 0306 and 0307.

Disclaimer: 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. We as supplier shall not be held liable for any