

## Chemical Safety Data Sheet MSDS / SDS

## 3-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: 3-nitroaniline  
CAS: 99-09-2

**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: 3-nitroaniline

Common names and synonyms: 3-nitroaniline

CAS number: 99-09-2

EC number: 202-729-1

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**

**SYMPTOMS:** Symptoms of exposure to this compound may include cyanosis and liver damage. When inhaled or ingested, this compound may cause headache, flushing of the face, difficult breathing, nausea, vomiting, weakness, drowsiness, irritability and dermatitis. Structurally similar chemicals may cause methemoglobinemia. **ACUTE/CHRONIC HAZARDS:** This chemical is a highly toxic irritant. It may be fatal if inhaled or swallowed. It causes eye and skin irritation. When heated to decomposition this compound emits toxic fumes of carbon monoxide, carbon dioxide and oxides of nitrogen. (NTP, 1992)

### **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**

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

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

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

### **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. Carefully collect remainder.

### 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. Carefully collect remainder.

### 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. Nitroaniline

## 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. Protect against physical damage to containers and prevent from moisture contacts.

## SECTION 8: Exposure controls/personal protection

### Control parameters

### Occupational Exposure limit values

Component	3-nitroaniline			
CAS No.	99-09-2			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m <sup>3</sup>	ppm	mg/m <sup>3</sup>

Finland	1	5,7	3 (1)	17 (1)
Latvia	?	0,1	?	?
	<b>Remarks</b>			
Finland	(1) 15 minutes average value			

### 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: PHYSICAL DESCRIPTION: Yellow needles or yellow powder. (NTP, 1992)

Colour: Yellow crystals from water

Odour: Burning sweet odor

Melting point/freezing point: 114 °C

Boiling point or initial boiling point and boiling range:	306 (broken down)
Flammability:	Combustible. Many reactions may cause fire or explosion.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	196 °C
Auto-ignition temperature:	no data available
Decomposition temperature:	306 °C
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Insoluble in water
Partition coefficient n-octanol/water:	log Kow = 1.37
Vapour pressure:	1 mm Hg ( 119 °C)
Density and/or relative density:	1.4
Relative vapour density:	no data available
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

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**

Dust explosion possible if in powder or granular form, mixed with air. Thermal stability of this compound is reduced by various impurities. This compound may be sensitive to prolonged exposure to light. This compound may react explosively with ethylene oxide at 266° F. It is incompatible with acids (nitric, sulfuric), acid chlorides, acid anhydrides, chloroformates and strong oxidizing agents. (NTP, 1992). Unstable when heated.

#### **Conditions to avoid**

no data available

#### **Incompatible materials**

Possibly explosive reaction with ethylene oxide at 130 deg C.

#### **Hazardous decomposition products**

When heated to decomp it emits toxic fumes of /nitrogen oxides/.

### **SECTION 11: Toxicological information**

#### **Acute toxicity**

Oral: LD50 Rat oral, SD strain (M), 540 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**

The substance may cause effects on the blood. This may result in the formation of methaemoglobin. Medical observation is indicated. The effects may be delayed. 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**

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

## **SECTION 12: Ecological information**

### **Toxicity**

Toxicity to fish: LC50; Species: Danio rerio (Zebra danio, age 3 months, weight 200-350 mg); Conditions: freshwater, renewal, 26.5 deg C, pH 8.6, dissolved oxygen 85%; Concentration: 594 umol/L for 96 hr

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: *Daphnia magna* (Water flea, 24 hr); Conditions: freshwater, static, 18-20 deg C, pH 8.0-8.3, dissolved oxygen 8.1-9.7 mg/L; Concentration: 6770 ug/L for 24 hr (95% confidence interval: 3990-11000 ug/L); Effect: intoxication, immobilization />98% purity

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

### **Persistence and degradability**

AEROBIC: The mono-nitroanilines were found to be markedly more resistant to biological degradation, as compared to aniline, using Warburg respirometer procedures(1). 3-Nitroaniline was determined to be non-biodegradable using the Japanese MITI protocol(2). No biodegradation of 3-nitroaniline (100 ppm) was observed in a 2-week period in the standard biodegradability test of the Japanese Ministry International Trade and Industry (MITI), a BOD test utilizing a mixed inoculum of activated sludge, sewage and surface water(3). No biodegradation of 3-nitroaniline was observed at concn of 25-30 ppm upon incubation with adapted activated sludge for 20 days(4). No degradation of 3-nitroaniline in a mineral salts solution, with a soil inoculum, occurred in 64 days(5). No biodegradation occurred over a 240 hr period in a respirometer study(6). Only limited biooxidation of 3-nitroaniline was observed in respirometric tests utilizing phenol-adapted bacteria(7). In a 60-day respirometer test using sewage seed, no biodegradation of 3-nitroaniline (5 ppm) occurred(8). However partial degradation was observed when the test solution was cross-seeded with microorganisms acclimated to 4-nitroaniline(8). Using the Zahn-Wellens test procedure, 3-nitroaniline was difficult to degrade as elimination was less than 20% over the 28 day incubation period(9). In another Zahn-Wellens test, no DOC removal occurred in 23 days of incubation(10). 3-Nitroaniline had a biodegradation rate of 0.026/h in river water giving a half-life of 27 hours, which was classified as poor degradation(11). A 5 day BOD at 20 deg C in Songhua river water was 6% for 3-nitroaniline(12).

### **Bioaccumulative potential**

A 6-week bioconcentration study in carp obtained BCF values of 1.1-3.0 and <10 for concentrations of 3- nitroaniline of 0.5 and 0.05 mg/L, respectively(1). An aquarium study using carp fish found 3-nitroaniline to have a low bioaccumulation potential(2). A study using zebrafish experimentally determined the BCF for 3-nitroaniline to be 8.3(3). According to a classification scheme(4), these BCF values suggest bioconcentration in aquatic organisms is low(SRC).

### **Mobility in soil**

Soil adsorption studies using four silt loam soils and a 2-hour adsorption period determined a mean log  $K_{om}$  of 1.70 which corresponds to a  $K_{oc}$  of 87 for 3-nitroaniline(1). 3-Nitroaniline had a measured log  $K_{oc}$  of 1.64 which corresponds to a  $K_{oc}$  value of 44(2). According to a classification scheme(3), these  $K_{oc}$  values suggest that 3-nitroaniline is expected to have very high to high mobility in soil(SRC). 3-Nitroaniline was found to have a  $K_d$  value of 3.5 L/kg in homoionic K<sup>+</sup> Montmorillonite type soil(4). However, anilines are expected to bind strongly to humus or organic matter in soils due to the high reactivity of the aromatic amino group(5,6), suggesting that mobility may be much lower in some soils(SRC).

### **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 0308.

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