

# SAFETY DATA SHEET

Version 6.6  
Revision Date 05/25/2023  
Print Date 11/11/2023

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

### 1.1 Product identifiers

Product name : 4-Nitroaniline  
Product Number : 185310  
Brand : Aldrich  
Index-No. : 612-012-00-9  
CAS-No. : 100-01-6

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Inhalation (Category 3), H331  
Acute toxicity, Dermal (Category 3), H311  
Specific target organ toxicity - repeated exposure (Category 2), H373  
Short-term (acute) aquatic hazard (Category 3), H402  
Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard statement(s)

H301 + H311 + H331  
H373

Toxic if swallowed, in contact with skin or if inhaled.  
May cause damage to organs through prolonged or repeated exposure.

H412

Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P260

Do not breathe dust.

P264

Wash skin thoroughly after handling.

P270

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

P271

Use only outdoors or in a well-ventilated area.

P273

Avoid release to the environment.

P280

Wear protective gloves/ protective clothing.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.  
Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

P304 + P340 + P311

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.

P314

Get medical advice/ attention if you feel unwell.

P362

Take off contaminated clothing and wash before reuse.

P403 + P233

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

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula :  $C_6H_6N_2O_2$   
Molecular weight : 138.12 g/mol  
CAS-No. : 100-01-6  
EC-No. : 202-810-1  
Index-No. : 612-012-00-9

Component	Classification	Concentration
<b>4-Nitroaniline</b>	Acute Tox. 3; STOT RE 2; Aquatic Acute 3; Aquatic Chronic 3; H301, H331, H311, H373, H402, H412	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

### 4.2 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

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

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

#### **5.4 Further information**

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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

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

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.  
For personal protection see section 8.

#### **6.2 Environmental precautions**

Do not let product enter drains.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

#### **6.4 Reference to other sections**

For disposal see section 13.

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

#### **7.1 Precautions for safe handling**

##### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

##### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

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

##### **Storage conditions**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Moisture sensitive.

##### **Storage class**

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

#### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
4-Nitroaniline	100-01-6	TWA	3 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	3 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	1 ppm 6 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		PEL	3 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

### 8.2 Exposure controls

#### Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested:KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested:KCL 741 Dermatril® L

### **Body Protection**

protective clothing

### **Respiratory protection**

required when dusts are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |
|---|---|
| a) Appearance                                   | Form: crystalline<br>Color: yellow                      |
| b) Odor   | Ammonia odor  |
| c) Odor Threshold                               | No data available                                       |
| d) pH   | 7.0   |
| e) Melting point/freezing point                 | Melting point/range: 146 - 149 °C (295 - 300 °F) - lit. |
| f) Initial boiling point and boiling range      | 260 °C 500 °F at 133 hPa - lit.                         |
| g) Flash point                                  | 213.0 °C (415.4 °F) - closed cup                        |
| h) Evaporation rate                             | No data available                                       |
| i) Flammability (solid, gas)                    | No data available                                       |
| j) Upper/lower flammability or explosive limits | No data available                                       |
| k) Vapor pressure                               | 0.005 hPa at 25.0 °C (77.0 °F)                          |
| l) Vapor density                                | No data available                                       |
| m) Density                                      | 1.44 g/cm <sup>3</sup>                                  |
| Relative density                                | No data available                                       |
| n) Water solubility                             | slightly soluble  |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.39log Pow: 5                                 |
| p) Autoignition temperature                     | 180.0 °C (356.0 °F)                                     |
| q) Decomposition temperature                    | No data available                                       |

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- r) Viscosity No data available
- s) Explosive properties No data available
- t) Oxidizing properties No data available

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Organic Substances

magnesium

Nitric acid

Exothermic reaction with:

sulfuric acid

Risk of explosion with:

Sodium hydroxide

organic nitro compounds

Ether

Violent reactions possible with:

strong reducing agents

Bases

Acid chlorides

Acid anhydrides

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitrosamines!

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

rubber, various plastics

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 750.0 mg/kg

LC50 Inhalation - 4 h - 0.51 mg/l - dust/mist

LD50 Dermal - Guinea pig - > 500.0 mg/kg

No data available

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

Remarks: No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### 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.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### Reproductive toxicity

No data available

Overexposure may cause reproductive disorder(s) based on tests with laboratory animals.

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

#### Aspiration hazard

No data available

### 11.2 Additional Information

RTECS: BY7000000

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer., Exposure to and/or consumption of alcohol may increase toxic effects., Headache, Unconsciousness, Cough, chest pain, Difficulty in breathing, Drowsiness, Nausea, Cyanosis, Ataxia., Diarrhea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated., p-Nitroaniline is readily absorbed by inhalation, ingestion, or skin absorption. It is a strong methemoglobin former. Cyanosis is the first manifestation of toxicity.

Liver -

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 85.7 - 142 mg/l - 96.0 h
	LC50 - Leuciscus idus (Golden orfe) - 35 mg/l - 48.0 h
	LC50 - Danio rerio (zebra fish) - 87.6 mg/l - 96.0 h
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 17.00 mg/l - 48 h
Toxicity to algae	EC50 - No information available. - 68.00 mg/l - 24 h

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

Bioaccumulation Danio rerio (zebra fish) - 96 h  
- 0.028 mg/l(4-Nitroaniline)

Bioconcentration factor (BCF): 4.4

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1661 Class: 6.1

Packing group: II

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Proper shipping name: Nitroanilines  
Reportable Quantity (RQ): 5000 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1661 Class: 6.1 Packing group: II EMS-No: F-A, S-A  
Proper shipping name: NITROANILINES (o-, m-, p-)

**IATA**

UN number: 1661 Class: 6.1 Packing group: II  
Proper shipping name: Nitroanilines

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**SECTION 15: Regulatory information**

**SARA 302 Components**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
4-Nitroaniline	100-01-6	2013-02-08

**SARA 311/312 Hazards**

Acute Health Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
4-Nitroaniline	100-01-6	2013-02-08

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
4-Nitroaniline	100-01-6	2013-02-08

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**SECTION 16: Other information**

**Further information**

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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