

## SAFETY DATA SHEET

Version 6.6  
Revision Date 11/27/2021  
Print Date 05/28/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-Nitrobenzoic acid

Product Number : 185329  
Brand : Aldrich  
CAS-No. : 121-92-6

**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)**

Eye irritation (Category 2A), H319

Short-term (acute) aquatic hazard (Category 3), H402

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

Warning

Hazard statement(s)

H319

Causes serious eye irritation.

H402

Harmful to aquatic life.

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Precautionary statement(s) |                                                                                                                                  |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P273                       | Avoid release to the environment.                                                                                                |
| P280                       | Wear 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. Continue rinsing. |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| 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 <sub>7</sub> H <sub>5</sub> NO <sub>4</sub> |
| Molecular weight | : 167.12 g/mol                                  |
| CAS-No.          | : 121-92-6                                      |
| EC-No.           | : 204-508-5                                     |

| Component                            | Classification                             | Concentration |
|--------------------------------------|--------------------------------------------|---------------|
| <b>m-Nitrobenzenecarboxylic acid</b> |                                            |               |
|                                      | Eye Irrit. 2A; Aquatic Acute 3; H319, H402 | <= 100 %      |

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

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air.

#### In case of skin contact

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

#### In case of eye contact

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

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### 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**

In the event of fire, wear self-contained breathing apparatus.

#### **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 inhalation of dusts. 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 dry. 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**

For precautions see section 2.2.

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

##### **Storage conditions**

Tightly closed. Dry.

### **Storage class**

Storage class (TRGS 510): 11: Combustible Solids

### **7.3 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**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

Change contaminated clothing. Wash hands 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: solid<br>Color: light yellow                                             |
| b) Odor                                         | No data available                                                              |
| c) Odor Threshold                               | No data available                                                              |
| d) pH                                           | ca.3 at 5 g/l                                                                  |
| e) Melting point/freezing point                 | Melting point/range: 139 - 141 °C (282 - 286 °F) - lit.                        |
| f) Initial boiling point and boiling range      | > 260 °C > 500 °F at 979.8 hPa - OECD Test Guideline 103                       |
| g) Flash point                                  | 189.6 °C (373.3 °F) - Pensky-Martens 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                               | No data available                                                              |
| l) Vapor density                                | No data available                                                              |
| m) Density                                      | 1.46 g/cm <sup>3</sup> at 20 °C (68 °F) at 978.4 hPa - OECD Test Guideline 109 |
| Relative density                                | No data available                                                              |
| n) Water solubility                             | ca.3 g/l at 25 °C (77 °F) - soluble                                            |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.1 at 25 °C (77 °F) - Bioaccumulation is not expected.               |
| p) Autoignition temperature                     | No data available                                                              |
| q) Decomposition temperature                    | No data available                                                              |
| r) Viscosity                                    | No data available                                                              |
| s) Explosive properties                         | No data available                                                              |
| t) Oxidizing properties                         | none                                                                           |

#### 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**

Violent reactions possible with:

Strong oxidizing agents

Bases

Risk of explosion with:

Potassium hydroxide

### **10.4 Conditions to avoid**

Strong heating.

### **10.5 Incompatible materials**

No data available

### **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 - female - > 2,000 mg/kg

(OECD Test Guideline 423)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Inhalation: No data available

LD50 Dermal - Rat - female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

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

Skin - reconstructed human epidermis (RhE)

Result: No skin irritation - 1 h

(OECD Test Guideline 439)

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

Eyes - In vitro study

Result: Irritating to eyes. - 6 h

(OECD Test Guideline 492)

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

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

#### **Germ cell mutagenicity**

Aldrich - 185329

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Test Type: Ames test  
Test system: *S. typhimurium*  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 471  
Result: negative  
Test Type: Chromosome aberration test in vitro  
Test system: Chinese hamster ovary cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 473  
Result: negative

Test Type: Mutagenicity (mammal cell test): micronucleus.  
Species: Mouse  
Cell type: Red blood cells (erythrocytes)  
Application Route: Oral

Result: negative  
Remarks: (National Toxicology Program)

### **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

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

Repeated dose toxicity - Rat - male - Oral - 42 Days - NOAEL (No observed adverse effect level) - 20 mg/kg

RTECS: DH5000000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

The following applies to aromatic nitro compounds in general: systemic effect: methaemoglobinaemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

|                                                     |                                                                                                                   |
|-----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | LC50 - <i>Oryzias latipes</i> - 50 mg/l - 96 h<br>Remarks: (External MSDS)                                        |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - <i>Daphnia magna</i> (Water flea) - 71.3 mg/l - 48 h<br>(OECD Test Guideline 202)              |
| Toxicity to algae                                   | static test ErC50 - <i>Desmodesmus subspicatus</i> (green algae) - 106.4 mg/l - 72 h<br>(OECD Test Guideline 201) |

### 12.2 Persistence and degradability

|                                 |                                                                        |
|---------------------------------|------------------------------------------------------------------------|
| Biodegradability                | Result: 73.33 % - Readily biodegradable.<br>(OECD Test Guideline 301D) |
| Biochemical Oxygen Demand (BOD) | 6.39 mg/g                                                              |
| Chemical Oxygen Demand (COD)    | 47.7 mg/g                                                              |

### 12.3 Bioaccumulative potential

|                 |                                                                                                                                   |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------|
| Bioaccumulation | Cyprinus carpio (Carp) - 6 Weeks<br>at 25 °C - 0.03 mg/l(m-Nitrobenzenecarboxylic acid)<br><br>Bioconcentration factor (BCF): 7.1 |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------|

### 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

|                                   |                                                                                                                                                                                               |
|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Additional ecological information | Depending on the concentration, phosphorus and/or nitrogen compounds may contribute to the eutrophication of drinking- water supplies.<br><br>Discharge into the environment must be avoided. |
|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

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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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

#### Further information

Not classified as dangerous in the meaning of transport regulations.

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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

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

#### SARA 311/312 Hazards

Acute Health Hazard

#### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know Components

|                               |                     |               |
|-------------------------------|---------------------|---------------|
| m-Nitrobenzenecarboxylic acid | CAS-No.<br>121-92-6 | Revision Date |
|-------------------------------|---------------------|---------------|

#### New Jersey Right To Know Components

|                               |                     |               |
|-------------------------------|---------------------|---------------|
| m-Nitrobenzenecarboxylic acid | CAS-No.<br>121-92-6 | Revision Date |
|-------------------------------|---------------------|---------------|

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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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