

## SAFETY DATA SHEET

Version 6.7  
Revision Date 09/06/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Nicotinic acid-(*ring*-d<sub>4</sub>)

Product Number : 486086  
Brand : Aldrich  
CAS-No. : 66148-15-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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 Statements

H319

Causes serious eye irritation.

H402

Harmful to aquatic life.

Precautionary Statements

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

Synonyms : 3-Pyridine-d4-carboxylic acid  
Niacin-d4 (ring-d4)

Formula : C<sub>6</sub>D<sub>4</sub>HNO<sub>2</sub>  
Molecular weight : 127.05 g/mol  
CAS-No. : 66148-15-0  
EC-No. : 689-511-3

Component	Classification	Concentration
<b>Nicotinic acid-ring-d4</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.

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**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.

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.

Light sensitive.

#### **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 EN 16523-1 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 EN 16523-1 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**

Recommended Filter type: Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.  
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: powder<br>Color: white                             |
| b) Odor                                    | No data available  |
| c) Odor Threshold                          | No data available  |
| d) pH                                      | No data available  |
| e) Melting point/freezing point            | Melting point/ range: 236 - 239 °C (457 - 462 °F) - lit. |
| f) Initial boiling point and boiling range | No data available  |
| g) Flash point                             | ( )Not applicable  |
| h) Evaporation rate                        | No data available  |
| i) Flammability (solid, gas)               | No data available  |
| j) Upper/lower                             | No data available  |

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flammability or  
explosive limits

- |  |  |
|--|--|
| k) Vapor pressure                            | No data available  |
| l) Vapor density                             | No data available  |
| m) Density                                   | No data available  |
| Relative density                             | No data available  |
| n) Water solubility                          | No data available  |
| o) Partition coefficient:<br>n-octanol/water | log Pow: -0.590 at 25 °C (77 °F) - Bioaccumulation is not<br>expected. |
| p) Autoignition<br>temperature               | No data available  |
| q) Decomposition<br>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

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:

Oxidizing agents  
bases  
acids

### 10.4 Conditions to avoid

no information available

### 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 - 7,000 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: nicotinic acid

LC50 Inhalation - Rat - male and female - 4 h - > 3.8 mg/l - Aerosol

(OECD Test Guideline 436)

Remarks: The value is given in analogy to the following substances: nicotinic acid

Symptoms: Possible damages: mucosal irritations

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

(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: nicotinic acid

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: nicotinic acid

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: nicotinic acid

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: nicotinic acid

#### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Remarks: The value is given in analogy to the following substances: nicotinic acid

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: nicotinic acid

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

Remarks: The value is given in analogy to the following substances: nicotinic acid  
Test Type: unscheduled DNA synthesis assay  
Test system: rat hepatocytes  
Method: OECD Test Guideline 482  
Result: negative  
Remarks: The value is given in analogy to the following substances: nicotinic acid  
Test Type: Micronucleus test  
Test system: Chinese hamster ovary cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 487  
Result: negative  
Remarks: The value is given in analogy to the following substances: nicotinic acid  
Test Type: Chromosome aberration test  
Species: Rat  
Cell type: Bone marrow  
Application Route: Oral  
Method: OECD Test Guideline 475  
Result: negative  
Remarks: The value is given in analogy to the following substances: nicotinic acid

### **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 and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 50 mg/kg

Remarks: The value is given in analogy to the following substances: nicotinic acid

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

Systemic effects:

After absorption of toxic quantities:

CNS disorders



narcosis  
vasodilation  
Nausea  
Vomiting  
drop in blood pressure  
collapse

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	static test LC50 - <i>Salmo trutta</i> - 520 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: nicotinic acid
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 77 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: nicotinic acid
Toxicity to algae	static test ErC50 - <i>Desmodesmus subspicatus</i> (green algae) - 105.6 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: nicotinic acid  static test NOEC - <i>Desmodesmus subspicatus</i> (green algae) - 25 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: nicotinic acid
Toxicity to bacteria	static test EC50 - <i>Pseudomonas putida</i> - 120 mg/l - 16 h (OECD Test Guideline 209) Remarks: The value is given in analogy to the following substances: nicotinic acid

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 14 d Result: 100 % - Readily biodegradable. (OECD Test Guideline 301E) Remarks: The value is given in analogy to the following substances:
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### **12.3 Bioaccumulative potential**

No data available

### **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)**

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**

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

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**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

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

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : 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.

**US State Regulations****Massachusetts Right To Know**

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

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

**TSCA** : Product contains substance(s) not listed on TSCA inventory.

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information****Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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Details in analogy to the undeuterated compound.

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