

## SAFETY DATA SHEET

Version 5.3  
Revision Date 05/23/2016  
Print Date 10/16/2019

---

1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 4-Nitrophenol-1,2,6-<sup>13</sup>C<sub>3</sub>

Product Number : 655686  
Brand : Aldrich  
Index-No. : 609-015-00-2

CAS-No. : 93628-02-5

## 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

---

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 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Specific target organ toxicity - repeated exposure (Category 2), H373

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)

H302 + H312 + H332

H373

Harmful if swallowed, in contact with skin or if inhaled

May cause damage to organs through prolonged or repeated exposure.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

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.

P280

Wear protective gloves/ protective clothing.

P301 + P312

IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P314	Get medical advice/ attention if you feel unwell.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P363	Wash contaminated clothing before reuse.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Chemical characterization	: Isotopically labeled
Formula	: $^{13}\text{C}_3\text{C}_3\text{H}_5$
Molecular weight	: 80.08 g/mol
CAS-No.	: 93628-02-5
Index-No.	: 609-015-00-2

#### Hazardous components

Component	Classification	Concentration
<b>4-Nitrophenol-1,2,6-<math>^{13}\text{C}_3</math></b>		
	Acute Tox. 4; STOT RE 2; H302 + H312 + H332, H373	<= 100 %

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

---

### 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

For personal protection see section 8.

#### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### 6.4 Reference to other sections

For disposal see section 13.

---

### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

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

Keep container tightly closed in a dry and well-ventilated place.

Store under inert gas. hygroscopic

#### 7.3 Specific end use(s)

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

---

### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

##### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

#### 8.2 Exposure controls

##### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

##### Personal protective equipment

###### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

###### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

###### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

###### Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

###### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	4.4 at 5 g/l at 24 °C (75 °F)
e) Melting point/freezing point	Melting point/range: 113 - 115 °C (235 - 239 °F) Melting point/range: 113 - 115 °C (235 - 239 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	169 °C (336 °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) Vapour pressure	9.2 hPa (6.9 mmHg) at 165 °C (329 °F) 0.8 hPa (0.6 mmHg) at 120 °C (248 °F)
l) Vapour density	No data available
m) Relative density	1.479 g/cm <sup>3</sup> at 20 °C (68 °F)
n) Water solubility	ca.15 g/l
o) Partition coefficient: n-octanol/water	log Pow: 1.91
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
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

---

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available  
In the event of fire: see section 5

---

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

#### Reproductive toxicity

No data available

No data available

#### 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

#### Additional Information

RTECS: Not available

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., Depending on the intensity and duration of exposure, effects may vary from mild irritation to severe destruction of tissue., Damage to the eyes.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

---

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

### 12.2 Persistence and degradability

No data available

### 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 Other adverse effects

No data available

---

### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

##### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

##### Contaminated packaging

Dispose of as unused product.

---

### 14. TRANSPORT INFORMATION

#### DOT (US)

UN number: 1663 Class: 6.1

Packing group: III

Proper shipping name: Nitrophenols

Reportable Quantity (RQ): 100 lbs

Poison Inhalation Hazard: No

#### IMDG

UN number: 1663 Class: 6.1

Packing group: III

EMS-No: F-A, S-A

Proper shipping name: NITROPHENOLS (o-, m-, p-)

#### IATA

UN number: 1663 Class: 6.1

Packing group: III

Proper shipping name: Nitrophenols

---

### 15. REGULATORY INFORMATION

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### SARA 313 Components

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

	CAS-No.	Revision Date
4-Nitrophenol-1,2,6-13C3	93628-02-5	2007-07-01

#### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

#### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

---

### 16. OTHER INFORMATION

#### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H312	Harmful in contact with skin.

H332 Harmful if inhaled.  
H373 May cause damage to organs through prolonged or repeated exposure.

**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

**Further information**

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.  
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.

**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 5.3

Revision Date: 05/23/2016

Print Date: 10/16/2019