

# • SAFETY DATA SHEET

Version 6.12  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 4-Nitrophenol  
Product Number : 1048  
Brand : Sigma-Aldrich  
Index-No. : 609-015-00-2  
CAS-No. : 100-02-7

### 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 number

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

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## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied


Acute toxicity (Oral) : Category 4

Acute toxicity (Inhalation) : Category 4  
Acute toxicity (Dermal) : Category 4  
Specific target organ toxicity - repeated exposure (Oral) : Category 2 (Kidney, Liver)  
Short-term (acute) aquatic hazard : Category 3

**Other hazards**

None known.

**GHS label elements**

Hazard pictograms : 

Signal word : Warning

Hazard statements : H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.  
H373 May cause damage to organs (Kidney, Liver) through prolonged or repeated exposure if swallowed.  
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**  
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.  
**Response:**  
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.  
P302 + P352 + P312 IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.  
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.  
P314 Get medical advice/ attention if you feel unwell.  
P363 Wash contaminated clothing before reuse.

**Disposal:**

P501 Dispose of contents/ container to an approved

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 100-02-7

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4-Nitrophenol	100-02-7*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

**SECTION 4. FIRST AID MEASURES**

- General advice : Show this 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. Consult a physician.
- 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.
- 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
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

**SECTION 5. FIREFIGHTING MEASURES**

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.
Specific hazards during fire fighting	:	Combustible.  Vapours 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.
Hazardous combustion products	:	Carbon oxides  Nitrogen oxides (NO <sub>x</sub> )
Specific extinguishing methods	:	No data available
Further information	:	Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation.
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Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

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.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

Further information on storage conditions : Tightly closed.  
Dry.  
Keep in a well-ventilated place.  
Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

Recommended storage temperature : Recommended storage temperature see product label.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

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.

Recommended Filter : Filter type P2  
type:

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.

Hand protection

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Full contact  
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatril® L

Remarks : 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)).

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

Skin and body protection : protective clothing

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

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**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Appearance : crystalline

Color : yellow

Odor : characteristic

Odor Threshold : No data available  
pH : 4.4 (75.2 °F / 24.0 °C)  
Concentration: 5.00000 g/l

Melting point/ range : 230 - 239 °F / 110 - 115 °C  
Method: lit.

Boiling point/boiling range : 534 °F / 279 °C  
Method: lit.

Flash point : 336.2 °F / 169.0 °C  
Method: closed cup

Evaporation rate : No data available

Burning rate : No data available

Self-ignition : 541.4 °F / 283.0 °C

Upper explosion limit /  
Upper flammability limit : No data available

Lower explosion limit /  
Lower flammability limit : No data available

Vapor pressure : 6.9 mmHg (329.0 °F / 165.0 °C)  
0.6 mmHg (248.0 °F / 120.0 °C)

Relative vapour density : No data available

Relative density : No data available

Density : 1.48 g/cm<sup>3</sup> (68 °F / 20 °C)

Solubility(ies)  
Water solubility : 14.8 g/l (77 °F / 25 °C)

Partition coefficient: n-  
octanol/water : log Pow: 1.95  
Method: OECD Test Guideline 117  
Bioaccumulation is not expected.

Autoignition temperature : 950 °F / 510 °C

Decomposition  
temperature : > 536 °F / > 280 °C

Viscosity

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Viscosity, dynamic	: 2.560 Pas (249.80 °F / 121.00 °C)
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Method: Regulation (EC) No. 440/2008, Annex, A.14 Not classified as explosive.
Oxidizing properties	: Method: Regulation (EC) No. 440/2008, Annex, A.17 none
Molecular weight	: 139.11 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

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.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Risk of explosion with: Reducing agents conc. sulfuric acid Risk of ignition or formation of inflammable gases or vapours with: alkalines alkali hydroxides
Conditions to avoid	: Strong heating.
Incompatible materials	: No data available
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 - 667 mg/kg

Remarks: (ECHA)

LC50 Inhalation - Rat - 4 h - 4.7 mg/l - dust/mist

Remarks: (External MSDS)

LD50 Dermal - Rat - 1,024 mg/kg

Remarks: (RTECS)

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

#### 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.

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 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

Ingestion - May cause damage to organs through prolonged or repeated exposure.

- Kidney, Liver

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

#### Aspiration hazard

No data available

### 11.2 Additional Information

RTECS: SM2275000

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

Eyes -

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **4-Nitrophenol:**

Toxicity to fish	:	LC50 (Danio rerio (zebra fish)): 10.4 mg/l Exposure time: 96 h Method: OECD Test Guideline 203
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 22 mg/l Exposure time: 48 h Method: OECD Test Guideline 202
Toxicity to algae/aquatic plants	:	EC50 (Desmodesmus subspicatus (green algae)): 23.7 mg/l Exposure time: 96 h Remarks: (Lit.)
Toxicity to microorganisms	:	EC5 (Pseudomonas putida): 0.9 mg/l Exposure time: 16 h Remarks: (IUCLID)

### Ecotoxicology Assessment

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

### Persistence and degradability

#### Components:

##### **4-Nitrophenol:**

Biodegradability	:	Result: Readily biodegradable. Biodegradation: 97 % Exposure time: 14 d Method: OECD Test Guideline 301A
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### Bioaccumulative potential

#### Components:

##### **4-Nitrophenol:**

Bioaccumulation	:	Species: Pimephales promelas (fathead minnow) Bioconcentration factor (BCF): 280
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Exposure time: 28 d  
Concentration: 0.0441 mg/l

Partition coefficient: n- : log Pow: 1.95  
octanol/water : Method: OECD Test Guideline 117  
Remarks: Bioaccumulation is not expected.

### **Mobility in soil**

No data available

### **Other adverse effects**

#### **Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

#### **Components:**

##### **4-Nitrophenol:**

Additional ecological : Do not empty into drains.  
information

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## **SECTION 13. DISPOSAL CONSIDERATIONS**

### **Disposal methods**

Waste from residues : 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**

### **International Regulations**

#### **IATA-DGR**

UN/ID No. : UN 1663  
Proper shipping name : Nitrophenols  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo : 677  
aircraft)  
Packing instruction : 670  
(passenger aircraft)

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**Millipore  
Sigma**

**IMDG-Code**

UN number : UN 1663  
 Proper shipping name : NITROPHENOLS (o-, m-, p-)

Class : 6.1  
 Packing group : III  
 Labels : 6.1  
 EmS Code : F-A, S-A  
 Marine pollutant : no

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations****49 CFR Road**

UN/ID/NA number : UN 1663  
 Proper shipping name : Nitrophenols

Class : 6.1  
 Packing group : III  
 Labels : Division 6.1 - Toxic substances  
 ERG Code : 153  
 Marine pollutant : no

Poison Inhalation Hazard : No

**Special precautions for user**

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

**SECTION 15. REGULATORY INFORMATION****CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
4-Nitrophenol	100-02-7	100	100

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

**Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

4-Nitrophenol 100-02-7 >= 90 - <= 100 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

**Clean Water Act**

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

4-Nitrophenol 100-02-7 >= 90 - <= 100 %

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product contains the following toxic pollutants listed under the U.S. Clean Water Act Section 307

4-Nitrophenol 100-02-7 >= 90 - <= 100 %

This product does not contain any priority pollutants related to the U.S. Clean Water Act

**US State Regulations**

**Massachusetts Right To Know**

4-Nitrophenol 100-02-7

**Pennsylvania Right To Know**

4-Nitrophenol 100-02-7

**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 components of this product are reported in the following inventories:**

TSCA : All substances listed as active on the 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.

## SECTION 16. OTHER INFORMATION

### Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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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