

# SAFETY DATA SHEET

Version 6.6  
Revision Date 03/04/2024  
Print Date 07/13/2024

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

### 1.1 Product identifiers

Product name : Pentachloronitrobenzene

Product Number : P8556

Brand : Sigma

Index-No. : 609-043-00-5

CAS-No. : 82-68-8

### 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)

Acute toxicity, Oral (Category 4), H302  
Skin sensitization (Category 1), H317  
Short-term (acute) aquatic hazard (Category 1), H400

Long-term (chronic) aquatic hazard (Category 1), H410

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

H302

Harmful if swallowed.

H317

May cause an allergic skin reaction.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P261

Avoid breathing dust.

P264

Wash skin thoroughly after handling.

P270

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

P272

Contaminated work clothing must not be allowed out of the workplace.

P273

Avoid release to the environment.

P280

Wear protective gloves.

P301 + P312 + P330

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

P302 + P352

IF ON SKIN: Wash with plenty of soap and water.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P363

Wash contaminated clothing before reuse.

P391

Collect spillage.

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 : PCNB  
Quintozene

Formula : C<sub>6</sub>Cl<sub>5</sub>NO<sub>2</sub>  
Molecular weight : 295.33 g/mol  
CAS-No. : 82-68-8  
EC-No. : 201-435-0  
Index-No. : 609-043-00-5

Component	Classification	Concentration
<b>Pentachloronitrobenzene</b>	Acute Tox. 4; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H302, H317, H400, H410	<= 100 %

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**MILLIPORE  
SIGMA**

	M-Factor - Aquatic Acute: 10	
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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

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. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. 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>)

Hydrogen chloride gas

Combustible.

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 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

Component	CAS-No.	Value	Control parameters	Basis
Pentachloronitrobenzene	82-68-8	TWA	0.5 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		

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## 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

Handle with impervious gloves.

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

#### 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     |
|               | Color: colorless |

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b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 140 - 143 °C (284 - 289 °F) - lit.
f) Initial boiling point and boiling range	328 °C 622 °F at 1,013 hPa
g) Flash point	No data available
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	1.718 g/cm <sup>3</sup> at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	insoluble
o) Partition coefficient: n-octanol/water	log Pow: 4.46
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

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

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Oxidizing agents

### 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 - 1,100 mg/kg

Inhalation: No data available

Dermal: No data available

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

#### 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

RTECS: DA6650000

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

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish LC50 - *Lepomis macrochirus* (Bluegill) - 0.1 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates EC50 - *Daphnia magna* (Water flea) - 0.77 mg/l - 48 h

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

Bioaccumulation *Oncorhynchus mykiss* (rainbow trout) - 36 d  
- 0.690 µg/l (Pentachloronitrobenzene)

Bioconcentration factor (BCF): 169

### 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. 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)**

UN number: 3077 Class: 9 Packing group: III  
Proper shipping name: Environmentally hazardous substance, solid, n.o.s.  
(Pentachloronitrobenzene)  
Reportable Quantity (RQ): 100 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 3077 Class: 9 Packing group: III EMS-  
No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.  
(Pentachloronitrobenzene)  
Marine pollutant : yes  
Marine pollutant : no

**IATA**

UN number: 3077 Class: 9 Packing group: III  
Proper shipping name: Environmentally hazardous substance, solid, n.o.s.  
(Pentachloronitrobenzene)

**Further information**

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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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
Pentachloronitrobenzene	82-68-8	2010-08-02

**SARA 311/312 Hazards**

Acute Health Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
Pentachloronitrobenzene	82-68-8	2010-08-02

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Pentachloronitrobenzene	82-68-8	2010-08-02

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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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