

## SAFETY DATA SHEET

Version 8.3  
Revision Date 10/26/2021  
Print Date 01/22/2022

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

Product name : 4-Pentylbromobenzene

Product Number : 646350  
Brand : Aldrich  
CAS-No. : 51554-95-1

**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)**

Skin irritation (Category 2), H315  
Serious eye damage (Category 1), H318  
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

Danger

Hazard statement(s)	
H315	Causes skin irritation.
H318	Causes serious eye damage.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash 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

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: 1-Bromo-4-pentylbenzene
Formula	: C <sub>11</sub> H <sub>15</sub> Br
Molecular weight	: 227.14 g/mol
CAS-No.	: 51554-95-1

Component	Classification	Concentration
<b>1-bromo-4-pentylbenzene</b>	Skin Irrit. 2; Eye Dam. 1; Aquatic Acute 1; Aquatic Chronic 1; H315, H318, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %

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.

**In case of eye contact**

After eye contact: rinse out with plenty of water. Immediately 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

Hydrogen bromide gas

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**

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: Do not breathe vapors, aerosols. 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 with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

### **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.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### **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**

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). Tightly fitting safety goggles

##### **Skin protection**

required

##### **Body Protection**

protective clothing

##### **Respiratory protection**

required when vapours/aerosols 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: liquid Color: colorless	
b) Odor	No data available	
c) Odor Threshold	No data available	
d) pH	No data available	
e) Melting point/freezing point	Melting point: -27 °C (-17 °F)	
f) Initial boiling point and boiling range	203 - 204 °C 397 - 399 °F - lit.	
g) Flash point	120 °C (248 °F) - c.c.	
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	0.005 hPa at 20 °C (68 °F) - OECD Test Guideline 104	
l) Vapor density	No data available	
m) Density	1.272 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.	
	Relative density	No data available
n) Water solubility	0.00014 g/l at 20 °C (68 °F) - OECD Test Guideline 105	
o) Partition coefficient: n-octanol/water	log Pow: > 5.7 at 25 °C (77 °F) - OECD Test Guideline 117 - Potential bioaccumulation	
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	No data available	

### 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.

## 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

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 - male and female - > 2,000 mg/kg  
(OECD Test Guideline 423)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritations

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### 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**

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                      static test LC50 - Danio rerio (zebra fish) - 0.8 mg/l - 96 h  
Remarks: (own results)

Toxicity to daphnia                      EC50 - Daphnia magna (Water flea) - 5.6 mg/l - 48 h  
and other aquatic                      (OECD Test Guideline 202)  
invertebrates                      Remarks: (above the solubility limit in the test medium)

Toxicity to algae                      EC50 - Desmodesmus subspicatus (green algae) - 0.4 mg/l - 72 h  
Remarks: (own results)

NOEC - Desmodesmus subspicatus (green algae) - 0.07 mg/l - 72 h  
Remarks: (own results)

### **12.2 Persistence and degradability**

Biodegradability                      Result: 0 % - Not readily biodegradable.  
Remarks: (own results)

### **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

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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)

NA-Number: 1993 Class: NONE Packing group: III  
Proper shipping name: Combustible liquid, n.o.s. (1-bromo-4-pentylbenzene)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (1-bromo-4-pentylbenzene)  
Marine pollutant : yes

### IATA

UN number: 3082 Class: 9 Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (1-bromo-4-pentylbenzene)

### 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

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

Fire 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

1-bromo-4-pentylbenzene	CAS-No. 51554-95-1	Revision Date
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### New Jersey Right To Know Components

1-bromo-4-pentylbenzene	CAS-No. 51554-95-1	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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