SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 4-Nitrobenzyl bromide

Product Number: N13054
Brand: Aldrich
CAS-No.: 100-11-8

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 corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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):
H314 Causes severe skin burns and eye damage.
H335 May cause respiratory irritation.

Precautionary statement(s)

P260 Do not breathe dusts or mists.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
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.
P363 Wash contaminated clothing before reuse.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS
Lachrymator.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: α-Bromo-4-nitrotoluene

Formula: C$_7$H$_6$BrNO$_2$
Molecular weight: 216.03 g/mol
CAS-No.: 100-11-8
EC-No.: 202-820-6

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
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</thead>
<tbody>
<tr>
<td>α-Bromo-4-nitrotoluene</td>
<td>Skin Corr. 1B; Eye Dam. 1; STOT SE 3; H314, H318, H335</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.
**If inhaled**
After inhalation: fresh air. Call in physician.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

**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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

### 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 (CO2) 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 (NOx)
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: 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.

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 (TRGS 510): 8A: Combustible, corrosive hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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
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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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**
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: solid
- **b)** Odor: No data available
- **c)** Odor Threshold: No data available
- **d)** pH: No data available
- **e)** Melting point/freezing point: Melting point/range: 96 - 99 °C (205 - 210 °F) - lit.
- **f)** Initial boiling point and boiling range: No data available
- **g)** Flash point: > 100 °C (> 212 °F)
- **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)** Relative density: No data available
- **n)** Water solubility: No data available
- **o)** Partition coefficient: n-octanol/water: No data available
- **p)** Autoignition: No data available
9.2 **Other safety information**
No data available

**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.
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
- Alcohols
- Amines

10.4 **Conditions to avoid**
- Avoid moisture.
- Strong heating.

10.5 **Incompatible materials**
- Mild steel

10.6 **Hazardous decomposition products**
In the event of fire: see section 5

**SECTION 11: Toxicological information**

11.1 **Information on toxicological effects**

**Acute toxicity**
Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Skin corrosion/irritation

Serious eye damage/eye irritation
Causes serious eye damage.

Respiratory or skin sensitization

Germ cell mutagenicity

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

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Aspiration hazard

11.2 Additional Information
RTECS: XS7967000

Cough, Shortness of breath, Headache, Nausea, Vomiting
Quantitative data on the toxicity of this product are not available.

Other information

The following applies to aromatic nitro compounds in general: systemic effect: methaemoglobinemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

Further data:

Handle in accordance with good industrial hygiene and safety practice.
SECTION 12: Ecological information

12.1 Toxicity
12.2 Persistence and degradability
12.3 Bioaccumulative potential
12.4 Mobility in soil
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
   Discharge into the environment must be avoided.

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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)
   UN number: 3261    Class: 8    Packing group: II
   Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (α-Bromo-4-nitrotoluene)
   Reportable Quantity (RQ):
   Poison Inhalation Hazard: No

IMDG
   UN number: 3261    Class: 8    Packing group: II    EMS-No: F-A, S-B
   Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (α-Bromo-4-nitrotoluene)

IATA
   UN number: 3261    Class: 8    Packing group: II
   Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (α-Bromo-4-nitrotoluene)

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**
Acute Health 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**

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**New Jersey Right To Know Components**

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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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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