SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 4-Nitrobenzoyl chloride
Product Number: 112208
Brand: Aldrich
CAS-No.: 122-04-3

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

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.
H318: Causes serious eye damage.
Precautionary statement(s)
P260 Do not breathe dusts or mists.
P264 Wash skin thoroughly after handling.
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): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Immediately call a POISON CENTER or doctor/ physician.
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.
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

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrobenzoyl chloride</td>
<td>Met. Corr. 1; Skin Corr. 1B; Eye Dam. 1; H290, H314, H318</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
Consult a physician. Show this material safety data sheet to the doctor in attendance.

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

In case of skin contact
Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.
In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

If swallowed
Do NOT induce vomiting. 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

SECTION 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
Carbon oxides
Nitrogen oxides (NOx)
Hydrogen chloride gas
Combustible.

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. 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
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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Avoid formation of dust and aerosols. **Advice on safe handling**
Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

**Advice on protection against fire and explosion**
Provide appropriate exhaust ventilation at places where dust is formed.

**Hygiene measures**
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
For precautions see section 2.2.

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

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

Moisture sensitive.

**Storage class**
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**
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**
Face shield and safety glasses 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.

**Full contact**
- Material: Nitrile rubber
- Minimum layer thickness: 0.11 mm
- Break through time: 480 min
- Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

**Splash contact**
- Material: Nitrile rubber
- Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**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**
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**
Do not let product enter drains.

---

**SECTION 9: Physical and chemical properties**

9.1 **Information on basic physical and chemical properties**

- **a) Appearance**
  - Form: crystalline
  - Color: yellowyellow
- **b) Odor**
  - stinging
- **c) Odor Threshold**
  - No data available
- **d) pH**
  - No data available
- **e) Melting point/freezing point**
  - Melting point/range: 71 - 74 °C (160 - 165 °F) - lit.
- **f) Initial boiling point and boiling range**
  - 202 - 205 °C 396 - 401 °F at 140 hPa - lit.
- **g) Flash point**
  - 102 °C (216 °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) Vapor pressure**
  - No data available
- **l) Vapor density**
  - No data available
- **m) Density**
  - No data available
Relative density: No data available
n) Water solubility: (decomposition)
o) Partition coefficient: log Pow: 1.25 - Bioaccumulation is not expected.
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
- Solubility in other solvents:
  - Alcohol at 20 °C (68 °F) - decomposes
  - Ether at 20 °C (68 °F) - soluble

SECTION 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: Avoid moisture.
10.5 Incompatible materials: Water, Alcohols, Oxidizing agents, Strong bases
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:
  - LD50 Oral - Rat: 5,600 mg/kg
  - Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.
  - LD50 Oral - Mouse: 3,440 mg/kg
  - Behavioral: Ataxia.
  - Behavioral: Muscle contraction or spasticity.
  - Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: damage of respiratory tract
  - Inhalation: Corrosive to respiratory system.
Dermal: No data available

**Skin corrosion/irritation**
Causes skin burns.

**Serious eye damage/eye irritation**
Causes serious eye damage.
Causes serious eye damage.

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: positive
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: Positive results were obtained in some in vitro tests.
Test Type: Mutagenicity (mammal cell test):
Result: negative
Remarks: (Lit.)

**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**
Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Decomposition of the substance with tissue moisture.

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).

Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 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
Discharge into the environment must be avoided.
Stability in water
Remarks: Hydrolyzes on contact with water.

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Product
Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

DOT (US)
UN number: 3261 Class: 8 Packing group: II
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-nitrobenzoyl chloride)
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. (4-nitrobenzoyl chloride)

IATA
UN number: 3261 Class: 8 Packing group: II
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-nitrobenzoyl chloride)
SECTION 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**
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.

**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**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrobenzoyl chloride</td>
<td>122-04-3</td>
<td></td>
</tr>
</tbody>
</table>

**New Jersey Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrobenzoyl chloride</td>
<td>122-04-3</td>
<td></td>
</tr>
</tbody>
</table>

SECTION 16: Other information

**Further information**
Copyright 2020 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.5                      Revision Date: 09/09/2021  Print Date: 08/12/2023