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

1.1 Product identifiers

Product name : 4-Nitrobenzenesulfonyl chloride
Product Number : 272248
Brand : Aldrich
CAS-No. : 98-74-8

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)

Serious eye damage (Category 1), H318
Skin sensitization (Sub-category 1A), H317
Reproductive toxicity (Category 2), H361

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)
H317 May cause an allergic skin reaction.
H318 Causes serious eye damage.
H361 Suspected of damaging fertility or the unborn child.

Precautionary statement(s)
P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing dust.
P272 Contaminated work clothing must not be allowed out of the workplace.
P280 Wear protective gloves/ protective clothing/ 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.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
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 - none

SECTION 3: Composition/information on ingredients

3.1 Substances
Formula : C₆H₄ClNO₄S
Molecular weight : 221.62 g/mol
CAS-No. : 98-74-8
EC-No. : 202-697-9

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-Nitrobenzenesulphonyl chloride</td>
<td>Eye Dam. 1; Skin Sens. 1A; Repr. 2; H318, H317, H361</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
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. Consult a physician.

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

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)
Sulfur oxides
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.

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.
  Moisture sensitive.

- **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**
  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**
Recommended Filter type: Filter type P3
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**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
</table>
| **a)** Appearance | Form: powder  
Color: light yellow  
| **b)** Odor | No data available  
| **c)** Odor Threshold | No data available  
| **d)** pH | No data available  
| **e)** Melting point/freezing point | Melting point/range: 66 - 70 °C (151 - 158 °F) - lit.  
| **f)** Initial boiling point and boiling range | 143 - 144 °C 289 - 291 °F at 2 hPa  
| **g)** Flash point | ()Not applicable  
| **h)** Evaporation rate | No data available  
| **i)** Flammability (solid, gas) | No data available  

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Aldrich - 272248
### Other safety information

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>0.00009 hPa at 20 °C (68 °F) - OECD Test Guideline 104</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>m) Density</td>
<td>No data available</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>No data available</td>
</tr>
<tr>
<td>o) Partition coefficient: n-octanol/water</td>
<td>log Pow: 2.1 at 20 °C (68 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.</td>
</tr>
<tr>
<td>p) Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>t) Oxidizing properties</td>
<td>none</td>
</tr>
</tbody>
</table>

### 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

Violent reactions possible with:

- Oxidizing agents
- Alkalis

#### 10.4 Conditions to avoid

Avoid moisture.

No information available

#### 10.5 Incompatible materials

Strong oxidizing agents

#### 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 - female - > 2,000 mg/kg (OECD Test Guideline 423)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Skin - human skin
Result: No skin irritation - 3 h (OECD Test Guideline 431)
Skin - human skin
Result: No skin irritation (OECD Test Guideline 439)

Serious eye damage/eye irritation
Eyes - Bovine cornea
Result: Irreversible effects on the eye (OECD Test Guideline 437)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: positive (OECD Test Guideline 429)

Germ cell mutagenicity
Test Type: Ames test
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 490
Result: equivocal evidence.
Test Type: Micronucleus test
Test system: Human lymphocytes
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 487
Result: negative

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**
Suspected of damaging fertility.

**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
Repeated dose toxicity - Rat - male and female - Gavage - NOAEL (No observed adverse effect level) - > 100 mg/kg

Cough, Shortness of breath, Headache, Nausea, Vomiting
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties cannot be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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**SECTION 12: Ecological information**

#### 12.1 Toxicity

| Toxicity to fish | static test LC50 - Cyprinus carpio (Carp) - > 100 mg/l - 96 h  
OECD Test Guideline 203 |
|------------------|---------------------------------------------------------------------|
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h  
OECD Test Guideline 202 |
| Toxicity to algae | static test ErC50 - Pseudokirchneriella subcapitata - > 100 mg/l - 72 h  
OECD Test Guideline 201 |
| static test NOEC - Pseudokirchneriella subcapitata - >= 100 mg/l - 72 h  
OECD Test Guideline 201 |
| Toxicity to bacteria | static test EC50 - activated sludge - > 1,000 mg/l - 30 h  
OECD Test Guideline 209 |

#### 12.2 Persistence and degradability

**Biodegradability**

- alcoholic - Exposure time 28 d
- Result: ca.3 % - Totally biodegradable  
OECD Test Guideline 301B

#### 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

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.

SECTION 14: Transport information

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

Further information
Not classified as dangerous in the meaning of transport regulations.

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.
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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