

SAFETY DATA SHEET

Version 6.12
Revision Date 09/07/2024
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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

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)**

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.

Aldrich - 272248

Page 1 of 11

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H317

May cause an allergic skin reaction.

H318

Causes serious eye damage.

H361

Suspected of damaging fertility or the unborn child.

Precautionary Statements

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 +

IF IN EYES: Rinse cautiously with water for several minutes.

P310

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 : $C_6H_4ClNO_4S$
Molecular weight : 221.62 g/mol
CAS-No. : 98-74-8
EC-No. : 202-697-9

| Component | Classification | Concentration |
|---|--|---------------|
| 4-Nitrobenzenesulphonyl chloride | | |
| | Eye Dam. 1; Skin Sens. 1A; Repr. 2; H318, H317, H361 | <= 100 % |

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 (NO_x)

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.

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

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 EN 16523-1 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 EN 16523-1 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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------|---------------------|
| 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 |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | 0.00009 hPa at 20 °C (68 °F) - OECD Test Guideline 104 0.0002 hPa at 25 °C(77 °F) - OECD Test Guideline 104 |
| l) Vapor density | No data available |
| m) Density | No data available |
| Relative density | 1.7420 °C - OECD Test Guideline 109 |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | log Pow: 2.1 at 20 °C (68 °F) - OECD Test Guideline 117 - 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

No data available

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

alkalines

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

Aldrich - 272248

Page 7 of 11

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 can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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) |

Aldrich - 272248

Page 8 of 11

| | |
|----------------------|--|
| 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 aerobic - 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**CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : 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.

US State Regulations**Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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

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