

3-Nitrobenzene sulfonic acid-sodium salt for synthesis

Revision: 21.09.2023

Product code: 25315

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

3-Nitrobenzene sulfonic acid-sodium salt for synthesis

CAS No: 127-68-4
Index No: 609-048-00-2
EC No: 204-857-3

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**

Reagents and laboratory chemicals
Only for laboratory and analysis purposes.

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Company name: AnalytiChem GmbH
ACD
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0 Telefax: 0203/5194-290
E-mail: info@analytichem.de
Contact person: Abteilung Produktsicherheit Telephone: 0203/5194-107/117
E-mail: produktsicherheit@analytichem.de
Internet: www.analytichem.de
Responsible Department: Abteilung Produktsicherheit

1.4. Emergency telephone number:

For Hazardous Materials [or Dangerous Goods] Incidents Spill, Leak, Fire, Exposure, or Accident Call CHEMTREC Day or Night Within USA and Canada: 1-800-424-9300 Outside USA and Canada: +1 703-741-5970 (collect calls accepted)

Further Information

A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Eye Irrit. 2; H319
Skin Sens. 1; H317

Full text of hazard statements: see SECTION 16.

2.2. Label elements**Regulation (EC) No 1272/2008****Signal word:** Warning**Pictograms:**

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Hazard statements

- H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.

Precautionary statements

- P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P302+P352 IF ON SKIN: Wash with plenty of water and soap.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: 3-(NO₂)C₆H₄SO₃Na
Molecular weight: 225,16 g/mol

Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
127-68-4	sodium 3-nitrobenzenesulphonate			100 %
	204-857-3	609-048-00-2		
	Eye Irrit. 2, Skin Sens. 1; H319 H317			

Full text of H and EUH statements: see section 16.

Further Information

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of = 0.1 % (w/w).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.

After contact with skin

Wash immediately with: Water
Take off immediately all contaminated clothing and wash it before reuse.
Call a physician immediately.

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.
Remove contact lenses, if present and easy to do. Continue rinsing.
Protect uninjured eye.

After ingestion

Rinse mouth immediately and drink plenty of water.
Call a physician immediately.

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4.2. Most important symptoms and effects, both acute and delayed

Irritant
Allergic reactions
Methaemoglobinaemia

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**

Co-ordinate fire-fighting measures to the fire surroundings.

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Combustible solids
Danger of dust explosion.
Hazardous combustion products
In case of fire may be liberated:
Sulphur oxides
Nitrogen oxides (NO_x)

5.3. Advice for firefighters

Avoid contact with skin, eyes and clothes.
In case of fire: Wear self-contained breathing apparatus.

Additional information

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.
Use water spray jet to protect personnel and to cool endangered containers.

SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****For non-emergency personnel**

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
Emergency procedures
Consult an expert
Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**For containment**

Cover drains.
Prevent spread over a wide area (e.g. by containment or oil barriers).
Collect in closed and suitable containers for disposal.
Take up carefully when dry. Take up dust-free and set down dust-free.

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

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Other information

- Provide adequate ventilation.
- Do not breathe dust/fume/gas/mist/vapours/spray.
- Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

- Safe handling: see section 7
- Personal protection equipment: see section 8
- Disposal: see section 13

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

- Read label before use. Handle and open container with care.
- Avoid dust formation. Do not breathe dust.
- When using do not eat, drink, smoke, sniff. Keep container tightly closed.
- Use personal protection equipment. Use extractor hood (laboratory).
- Provide adequate ventilation. Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

- Usual measures for fire prevention.

Advice on general occupational hygiene

- Keep away from food, drink and animal feedingstuffs. Make available sufficient washing facilities
- Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink.

Further information on handling

- Draw up and observe skin protection programme.
- Wash hands and face before breaks and after work and take a shower if necessary.
- Take off immediately all contaminated clothing and wash it before reuse.
- If handled uncovered, arrangements with local exhaust ventilation have to be used.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

- Keep container tightly closed.

Hints on joint storage

- national regulations

Further information on storage conditions

- Store in a dry place.
- storage temperature < +30°

7.3. Specific end use(s)

- Laboratory chemicals

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****8.2. Exposure controls****Appropriate engineering controls**

- Technical measures and the application of suitable work processes have priority over personal protection equipment.
- If handled uncovered, arrangements with local exhaust ventilation have to be used.
- Avoid dust formation. Do not breathe dust.

Individual protection measures, such as personal protective equipment

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Eye/face protection

goggles

Wear eye protection/face protection.

Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

Trade name/designation: KCL 741 Dermatril® L

Suitable material: NBR (Nitrile rubber) 0,11 mm

Wearing time with permanent contact: > 480 min

Trade name/designation: KCL 741 Dermatril® L

Suitable material: NBR (Nitrile rubber) 0,11 mm

Wearing time with occasional contact (splashes): > 480 min

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types. 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).

Skin protection

Wear suitable protective clothing.

Take off immediately all contaminated clothing.

Wash hands before breaks and after work.

The choice of body protection depends on the concentration and quantity of hazardous substances. The chemical resistance of protective agents must be clarified with their suppliers.

Respiratory protection

Respiratory protection necessary at: dust formation

Filtering device with filter or ventilator filtering device of type: P2

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.

Environmental exposure controls

Do not allow to enter into surface water or drains.

SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state:	solid
Colour:	yellow
Odour:	odourless
Odour threshold:	No data available
Melting point/freezing point:	350 °C
Boiling point or initial boiling point and boiling range:	No data available
Flammability:	No data available
Lower explosion limits:	No data available
Upper explosion limits:	No data available
Flash point:	No data available
Auto-ignition temperature:	355 °C
Decomposition temperature:	No data available
pH-Value (at 23 °C):	8 (50 g/l)

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Viscosity / kinematic:	No data available
Water solubility: (at 20 °C)	200 g/l
Solubility in other solvents	
No data available	
Dissolution rate:	No data available
Partition coefficient n-octanol/water:	log Pow: -2,61
Dispersion stability:	No data available
Vapour pressure:	No data available
Vapour pressure:	No data available
Density (at 20 °C):	0,45 g/cm ³
Relative density:	No data available
Bulk density:	450 kg/m ³
Relative vapour density:	No data available
Particle characteristics:	No data available

9.2. Other information**Information with regard to physical hazard classes**

Explosive properties

Danger of dust explosion.

Sustained combustibility:

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

100%

Sublimation point:

No data available

Softening point:

No data available

Pour point:

No data available

No data available:

Viscosity / dynamic:

No data available

Flow time:

No data available

Further Information

No data available

SECTION 10: Stability and reactivity**10.1. Reactivity**

Danger of dust explosion.

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 stable under storage at normal ambient temperatures.

10.3. Possibility of hazardous reactions

Oxidising agent

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10.4. Conditions to avoid

Heat

10.5. Incompatible materials

No data available

10.6. Hazardous decomposition products

In case of fire may be liberated:

SECTION 5: Firefighting measures

Further information

No data available

SECTION 11: Toxicological information**11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008****Toxicokinetics, metabolism and distribution**

No data available

Acute toxicity

Based on available data, the classification criteria are not met.

Mucous membrane irritation in the mouth, throat, esophagus and gastrointestinal tract.

Irritation and corrosivity

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

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Sensitising effects

May cause an allergic skin reaction. (sodium 3-nitrobenzenesulphonate)

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Additional information on tests

No data available

Practical experience

No data available

11.2. Information on other hazards**Endocrine disrupting properties**

No data available

Other information

No data available

Further information

Irritant

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Allergic reactions
Methaemoglobinaemia

SECTION 12: Ecological information**12.1. Toxicity**

No data available

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

log Pow: -2,61

No indication of bioaccumulation potential.

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

No data available

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

No data available

12.7. Other adverse effects

No data available

Further information

Do not allow to enter into surface water or drains.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.

Send to a physico-chemical treatment facility under observation of official regulations.

Do not allow to enter into surface water or drains.

Contaminated packaging

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information**Land transport (ADR/RID)****14.1. UN number or ID number:**

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)**14.1. UN number or ID number:**

No dangerous good in sense of this transport regulation.

14.2. UN proper shipping name:

No dangerous good in sense of this transport regulation.

14.3. Transport hazard class(es):

No dangerous good in sense of this transport regulation.

14.4. Packing group:

No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

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14.1. UN number or ID number:	No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name:	No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es):	No dangerous good in sense of this transport regulation.
14.4. Packing group:	No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	No dangerous good in sense of this transport regulation.
14.2. UN proper shipping name:	No dangerous good in sense of this transport regulation.
14.3. Transport hazard class(es):	No dangerous good in sense of this transport regulation.
14.4. Packing group:	No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Restrictions on use (REACH, annex XVII):

Entry 75

Information according to Directive
2012/18/EU (SEVESO III):

Not subject to 2012/18/EU (SEVESO III)

National regulatory information

Employment restrictions:

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D):

1 - slightly hazardous to water

SECTION 16: Other information**Changes**

This data sheet contains changes from the previous version in section(s): 9,11,12,13.

Abbreviations and acronyms

Eye Irrit. 2: Eye irritation, hazard category 2

Skin Sens. 1: Skin sensitisation, hazard category 1

Relevant H and EUH statements (number and full text)

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

Further Information

Provide appropriate information, instructions and training to users

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

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The receiver of our product is singularly responsible for adhering to existing laws and regulations.