



SAFETY DATA SHEET

3-Nitrobenzenesulfonic acid sodium salt

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

1.1. Product identifier

Product name	3-Nitrobenzenesulfonic acid sodium salt
Synonyms; trade names	Sodium 3-nitrobenzenesulfonate
CAS number	127-68-4
EC number	204-857-3

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

Identified uses	Research and development.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Eye Irrit. 2 - H319 Skin Sens. 1 - H317
Environmental hazards	Not Classified

2.2. Label elements

EC number	204-857-3
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Hazard pictograms



Signal word	Warning
Hazard statements	H319 Causes serious eye irritation. H317 May cause an allergic skin reaction.

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Precautionary statements	P261 Avoid breathing dust.
	P264 Wash contaminated skin thoroughly after handling.
	P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
	P302+P352 IF ON SKIN: Wash with plenty of water.
	P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
	P333+P313 If skin irritation or rash occurs: Get medical advice/ attention.
	P337+P313 If eye irritation persists: Get medical advice/ attention.
	P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	3-Nitrobenzenesulfonic acid sodium salt
CAS number	127-68-4
EC number	204-857-3
Chemical formula	O ₂ NC ₆ H ₄ SO ₃ Na

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if symptoms are severe or persist.
Ingestion	Rinse mouth thoroughly with water. Get medical advice/attention if you feel unwell. Do not induce vomiting unless under the direction of medical personnel.
Skin contact	It is important to remove the substance from the skin immediately. In the event of any sensitisation symptoms developing, ensure further exposure is avoided. Remove contamination with soap and water or recognised skin cleansing agent. Get medical attention if symptoms are severe or persist after washing.
Eye contact	Rinse with water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Get medical attention if any discomfort continues.
Protection of first aiders	First aid personnel should wear appropriate protective equipment during any rescue.

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

General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Temporary irritation.
Ingestion	May cause sensitisation or allergic reactions in sensitive individuals.
Skin contact	May cause skin sensitisation or allergic reactions in sensitive individuals. Prolonged contact may cause dryness of the skin.
Eye contact	Irritating to eyes.

4.3. Indication of any immediate medical attention and special treatment needed

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Notes for the doctor Treat symptomatically. May cause sensitisation or allergic reactions in sensitive individuals.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

Unsuitable extinguishing media Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards None known.

Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon. Oxides of nitrogen. Oxides of sulphur. Sodium oxides

5.3. Advice for firefighters

Protective actions during firefighting Avoid breathing fire gases or vapours. Evacuate area. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid contact with skin and eyes.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

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Usage precautions Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

Advice on general occupational hygiene Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions Store away from incompatible materials (see Section 10). Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage. Protect from moisture.

Storage class Chemical storage.

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

8.2. Exposure controls

Protective equipment



Appropriate engineering controls

Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

Hand protection

It is recommended that chemical-resistant, impervious gloves are worn. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.

Other skin and body protection

May cause skin sensitisation or allergic reactions in sensitive individuals. Wear appropriate clothing to prevent repeated or prolonged skin contact.

Hygiene measures

Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.

Respiratory protection

Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.

Environmental exposure controls

Keep container tightly sealed when not in use.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Crystalline powder.
Colour	Yellow-white.
Odour	Not known.
Odour threshold	No information available.
pH	pH (concentrated solution): 8.0 at 25°C/77°F
Melting point	350°C/662°F
Initial boiling point and range	577°C/1071°F @ 101325 Pa
Flash point	100°C / 212°F Method: Closed cup.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	10.3 Pa @ 25°C/77°F
Vapour density	No information available.
Relative density	1.87 g/cm ³ @ 23°C/73°F
Solubility(ies)	200 g/l water @ 25°C/77°F 2900 mg/l methanol @ 23°C/73°F
Partition coefficient	log Pow: -2.61
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

9.2. Other information

Molecular weight	225.15
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SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity	See the other subsections of this section for further details.
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10.2. Chemical stability

Stability	Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.
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10.3. Possibility of hazardous reactions

Possibility of hazardous reactions	No potentially hazardous reactions known.
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10.4. Conditions to avoid

Conditions to avoid	There are no known conditions that are likely to result in a hazardous situation.
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10.5. Incompatible materials

Materials to avoid	Strong oxidising agents. Cadmium. Copper. Nickel. Brass.
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10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

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

Acute toxicity - dermal

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

Acute toxicity - inhalation

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

Skin corrosion/irritation

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

Serious eye damage/irritation

Summary Causes serious eye irritation.

Respiratory sensitisation

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

Skin sensitisation

Summary May cause an allergic skin reaction.

Germ cell mutagenicity

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

Carcinogenicity

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

IARC carcinogenicity None of the ingredients are listed or exempt.

Reproductive toxicity

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

Specific target organ toxicity - single exposure

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

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

Summary Not relevant. Solid.

General information

The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation

A single exposure may cause the following adverse effects: Temporary irritation.

Ingestion

May cause sensitisation or allergic reactions in sensitive individuals.

Skin contact

May cause skin sensitisation or allergic reactions in sensitive individuals. Prolonged contact may cause dryness of the skin.

Eye contact

Irritating to eyes.

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Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.
Medical considerations	Skin disorders and allergies.

SECTION 12: Ecological information

Ecotoxicity	Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.
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12.1. Toxicity

Acute aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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Acute toxicity - fish	LC ₅₀ , 96 hours: 500 mg/l, <i>Leuciscus idus</i> (Golden orfe) LC ₅₀ , 48 hours: >1000 mg/l, <i>Oryzias latipes</i> (Red killifish)
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Acute toxicity - aquatic invertebrates	LC ₅₀ , 48 hours: 8665 mg/l, <i>Daphnia magna</i>
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Acute toxicity - aquatic plants	EC ₅₀ , 72 hours: 500 mg/l, <i>Desmodesmus subspicatus</i>
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Chronic aquatic toxicity

Summary	Based on available data the classification criteria are not met.
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12.2. Persistence and degradability

Persistence and degradability	The degradability of the product is not known.
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12.3. Bioaccumulative potential

Bioaccumulative potential	No data available on bioaccumulation.
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Partition coefficient	log Pow: -2.61
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12.4. Mobility in soil

Mobility	No data available.
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12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment	This product does not contain any substances classified as PBT or vPvB.
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12.6. Other adverse effects

Other adverse effects	None known.
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SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information	The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.
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Disposal methods	Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.
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SECTION 14: Transport information

General

The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).

14.1. UN number

Not applicable.

14.2. UN proper shipping name

Not applicable.

14.3. Transport hazard class(es)

No transport warning sign required.

14.4. Packing group

Not applicable.

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture**National regulations**

Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories**EU - EINECS/ELINCS**

None of the ingredients are listed or exempt.

SECTION 16: Other information

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Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
	ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
	RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
	IATA: International Air Transport Association.
	ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
	IMDG: International Maritime Dangerous Goods.
	CAS: Chemical Abstracts Service.
	ATE: Acute Toxicity Estimate.
	LC50: Lethal Concentration to 50 % of a test population.
	LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).
	EC ₅₀ : 50% of maximal Effective Concentration.
	PBT: Persistent, Bioaccumulative and Toxic substance.
	vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Eye Irrit. = Eye irritation
	Skin Sens. = Skin sensitisation
Classification procedures according to SI 2019 No. 720	Eye Irrit. 2 - H319: Skin Sens. 1 - H317: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	23/08/2022
Revision	1
SDS number	1369
Hazard statements in full	H317 May cause an allergic skin reaction.
	H319 Causes serious eye irritation.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.