

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



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

1.1. Product identifier

Trade name

5-Bromo-5-nitro-1,3-dioxane

CAS number

30007-47-7

EC number

250-001-7

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

Relevant identified uses

Research and development. Laboratory Chemicals. Manufacture of substances.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,
 DL1 4XX Darlington
 United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Hazardous to the aquatic environment — Acute hazard category 1
 Hazardous to the aquatic environment — Chronic hazard category 1
 Skin corrosion, hazard category 1A
 Specific Target Organ Toxicity — Repeated exposure, hazard category 2
 Acute toxicity, oral, hazard category 4
 Specific Target Organ Toxicity — Single exposure, hazard category 3

Hazard statements

H302, H314, H335, H373, H400, H410

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H302 Harmful if swallowed.
 H314 Causes severe skin burns and eye damage.
 H335 May cause respiratory irritation.
 H373 May cause damage to organs through prolonged or repeated exposure.
 H410 Very toxic to aquatic life with long lasting effects.

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Precautionary statements

P260 Do not breathe dust/fumes/gas/mist/vapours/spray.
 P264 Wash skin thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P271 Use only outdoors or in a well-ventilated area.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
 P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
 P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
 P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 P310 Immediately call a POISON CENTER/doctor.
 P363 Wash contaminated clothing before reuse.
 P391 Collect spillage.
 P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
 P405 Store locked up.
 P501 Dispose of contents/container to local regulations.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-pharse M factor acute M factor chronic	Note
5-Bromo-5-nitro-1,3-dioxane	30007-47-7 250-001-7 - -	100%	Acute Tox. 4 - oral, Skin Corr. 1A, STOT RE 2, Aquatic Acute 1, Aquatic Chronic 1, STOT SE 3	H302, H314, H335, H373, H400, H410 - -	-

Molecular weight

212.00

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

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SECTION 4: First aid measures

4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel. Chemical burns must be treated by a physician.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary. Maintain an open airway. Loosen any tight clothing, such as a collar, tie or belt. Get medical attention. Place unconscious person on the side in the recovery position and ensure breathing can take place.

Skin contact

Important to remove the substance from the skin immediately. Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes and get medical attention. Chemical burns must be treated by a physician.

Eye contact

Rinse immediately with plenty of water. Do not rub eye. Immediately flush with plenty of water for at least 15 minutes. Remove any contact lenses and open eyes wide apart. Continue to rinse for at least 15 minutes and get medical attention.

Ingestion

Rinse mouth thoroughly. Immediately give a couple of glasses of water or milk, provided the victim is fully conscious. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on the side in the recovery position and ensure breathing can take place. NOTE! Effects may be delayed. Keep affected person under observation. Get medical advice/attention.

Information for doctors

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

Inhalation

Single exposure may cause the following adverse effects: Severe irritation in nose and throat. Symptoms following overexposure may include the following: Corrosive to the respiratory tract.

Skin contact

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death. Redness.

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



Eye contact

Single exposure may cause the following adverse effects: Causes serious eye damage. Pain. Redness. Profuse watering of the eyes.

Ingestion

May cause chemical burns in mouth, oesophagus and stomach.
 Symptoms following overexposure may include the following: Severe abdominal pain. Nausea, vomiting.

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

Treat symptomatically. Immediately call a POISON CENTER/doctor.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish. Use fire-extinguishing media appropriate for surrounding materials.

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: Corrosive.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO₂).

Nitrous gases (NO_x).

Hydrogen bromide (HBr).

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



6.3. Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2. Do not handle until all safety precautions have been read and understood. Work under hood Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid discharge to the aquatic environment. Avoid contact with skin and eyes. Avoid ingestion and inhalation. Do not handle broken packages without protective equipment. Do not reuse empty containers.

General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.
 Store at ambient temperature.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

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5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



Hand protection

Wear protective gloves. Recommended gloves: Nitrile.

Glove Thickness: 0.11mm

Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Colour

No data available

Odour

No data available

Melting point / freezing point

59 - 961 °C

Boiling point or initial boiling point and boiling range

185.2 °C

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

No data available

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According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

No data available

Kinematic viscosity

No data available

Solubility

4.77 g/l

Partition coefficient n-octanol/water

log Pow: 1.6 at 23 °C - OECD Test Guideline 117 - Bioaccumulation is not expected.

Vapour pressure

0.34 hPa at 50 °C

Density and/or relative density

1.96 g/cm³

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Risk of dust explosion.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

Avoid generation and spreading of dust. Avoid dust close to ignition sources.

10.5. Incompatible materials

Strong oxidising agents.

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Test animals
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	LD50	455 mg/kg	Oral	Rat
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	LD50	455 mg/kg	Oral	Rat
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	LD50	455 mg/kg	Oral	Rat

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Species
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	Causes severe burns.	reconstructed human epidermis (RhE)
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	Causes severe burns.	reconstructed human epidermis (RhE)
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	Causes severe burns.	reconstructed human epidermis (RhE)

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Duration of exposure	Species	Other
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	CAUSES BURNS.	4 hours	Bovine cornea	Causes serious eye damage.
5-Bromo-5-nitro-1,3-dioxane	CAUSES BURNS.	4 hours	Bovine cornea	Causes serious eye damage.

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
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Replaces SDS: 2023-01-05



Product / Substance name CAS / EC no.	Result	Duration of exposure	Species	Other
30007-47-7 / 250-001-7				
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	CAUSES BURNS.	4 hours	Bovine cornea	Causes serious eye damage.

Aspiration hazard

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

11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity

Acute algae toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	EC10	0.088mg/l	72 hours	Pseudokirchneriella subcapitata
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	ErC50	0.265 mg/l	72 hours	Pseudokirchneriella subcapitata

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	EC50	1.32 mg/l	48 hours	Daphnia magna

12.2. Persistence and degradability

Persistence and degradability

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



Product / Substance name CAS / EC no.	Type of test	Duration	Result	Degradation
5-Bromo-5-nitro-1,3-dioxane 30007-47-7 / 250-001-7	aerobic	7 days	0%	The product is not readily biodegradable.

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

3261

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (5-Bromo-5-nitro-1,3-dioxane)

IMDG proper shipping name

CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (5-Bromo-5-nitro-1,3-dioxane)

IATA proper shipping name

Corrosive solid, acidic, organic, n.o.s. (5-Bromo-5-nitro-1,3-dioxane)

According to Regulation (EC) No 1907/2006

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Version number: 2
 Issued: 2024-01-25
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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



8

IMDG



8

IATA



8

ADR / RID Class

8

ADR / RID Classification code

C4

ADR / RID hazard identification number

80

IMDG Class

8

IATA Class

8

ADN Class

8

ADN Class Code

C4

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

5-Bromo-5-nitro-1,3-dioxane

Version number: 2
 Issued: 2024-01-25
 Replaces SDS: 2023-01-05



14.4. Packing group

ADR / RID / ADN: II

IMDG: II

IATA: II

14.5. Environmental hazards

IMDG EmS

F-A, S-B

14.6. Special precautions for user

Tunnel restriction code: E

Transport category: 2

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

SECTION 15: Regulatory information

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

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

Directive: 2012/18/EU: E1 ENVIRONMENTAL HAZARDS

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Aquatic Acute 1 - Hazardous to the aquatic environment — Acute hazard category 1

Aquatic Chronic 1 - Hazardous to the aquatic environment — Chronic hazard category 1

Skin Corr. 1A - Skin corrosion, hazard category 1A

STOT RE 2 - Specific Target Organ Toxicity — Repeated exposure, hazard category 2

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.

H373 May cause damage to organs through prolonged or repeated exposure.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.