Chemical Safety Data Sheet MSDS / SDS

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

Revision Date: 2024-12-21 Revision Number: 1

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

Product identifier

Product name : 5-Bromo-5-nitro-1,3-dioxane

CBnumber : CB3452622
CAS : 30007-47-7
EINECS Number : 250-001-7

Synonyms: BND,5-BROMO-5-NITRO-1,3-DIOXANE

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.

Uses advised against : none

Company Identification

Company : Chemicalbook

Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing

Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word Danger

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

 $P303 + P361 + P353 \; \text{IF ON SKIN (or hair)}: \; Remove/Take \; off \; Immediately \; \text{all contaminated clothing}. \; Rinse \; SKIN \; \text{with water/shower}.$

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thouroughly after handling.

P264 Wash hands thoroughly after handling.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

Hazard statements

H410 Very toxic to aquatic life with long lasting effects

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

H314 Causes severe skin burns and eye damage

H302 Harmful if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name : 5-Bromo-5-nitro-1,3-dioxane

Synonyms: BND,5-BROMO-5-NITRO-1,3-DIOXANE

CAS : 30007-47-7
EC number : 250-001-7
MF : C4H6BrNO4

MW : 212

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx) Hydrogen bromide gas Combustible.

Advice for firefighters

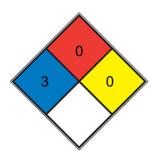
Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704

FIRE



Short exposure could cause serious temporary or moderate residual injury (e.g. <u>liquid hydrogen, sulfuric acid</u>, <u>calcium</u>

HEALTH 3

hypochlorite, hexafluorosilicic acid)

Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete,

0 stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)

SPEC.

☐ HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Reference to other sections

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min Material tested:Dermatril? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	solid
Odour	No data available
Odour Threshold	No data available
рН	No data available
Melting point/freezing point	Melting point: 59 °C at 1.013,25 hPa - OECD Test Guideline 102
Initial boiling point and boiling range	185,2 °C at 200 hPa - OECD Test Guideline 103
Flash point	No data available
Evaporation rate	No data available
Flammability (solid, gas)	The product is not flammable Test N.1: Test method for readily combustible solids
Upper/lower flammability or explosive	No data available
limits	
Vapour pressure	0,34 hPa at 50 °C - OECD Test Guideline 104
Vapour density	No data available
Relative density	1,96 at 20 °C - OECD Test Guideline 109
Water solubility	4,77 g/l at 20 °C - OECD Test Guideline 105
Partition coefficient: n-octanol/water	log Pow: 1,6 at 23 °C - OECD Test Guideline 117 - Bioaccumulation is not expected.
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available Chemical Book

Other safety information

Surface tension 71 mN/m at 1g/l at 20 °C

- OECD Test Guideline 115

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 455 mg/kg (OECD Test Guideline 401)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Behavioral:Tremor. Behavioral:Convulsions or effect on seizure threshold. Behavioral:Excitement.

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE) Result: Causes severe burns.

(OECD Test Guideline 431)

Serious eye damage/eye irritation

Eyes - Bovine cornea Result: Causes burns. - 4 h (OECD Test Guideline 437) Causes serious eye damage.

Respiratory or skin sensitization Germ cell mutagenicity 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.

Reproductive toxicity

Specific target organ toxicity - single exposure

Acute oral toxicity - If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Acute inhalation toxicity - mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure Aspiration hazard

SECTION 12: Ecological information

Toxicity

No data available

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 1,32 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae

static test ErC50 - Pseudokirchneriella subcapitata - 0,265 mg/l - 72 h

(OECD Test Guideline 201)

static test EC10 - Pseudokirchneriella subcapitata - 0,088 mg/l - 72 h

(OECD Test Guideline 201)

Persistence and degradability

Biodegradability aerobic - Exposure time 7 d

Result: 0 % - Not readily biodegradable. (OECD Test Guideline 301D)

Bioaccumulative potential

Mobility in soil

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Very toxic to aquatic life with long lasting effects.

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3261 IMDG: 3261 IATA: 3261

UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (5-bromo-5-nitro-1,3-dioxane) IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC,

N.O.S. (5-bromo-5-nitro-1,3-dioxane)

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

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

New Zealand Inventory of Chemicals (NZloC):Listed. website: https://www.epa.govt.nz/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit TWA: Time Weighted Average

References

[1] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

[2] ChemlDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

[3] ECHA - European Chemicals Agency, website: https://echa.europa.eu/

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

[6] Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

[7] HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

[8] IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

[9] IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

【10】 Sigma-Aldrich, website: https://www.sigmaaldrich.com/

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.