

Chemical Safety Data Sheet MSDS / SDS

9-BBN triflate

Revision Date:2026-09-12 Revision Number:1

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

Product identifier

Product name : 9-BBN triflate
CBnumber : CB2303895
CAS : 62731-43-5
Synonyms : 9-BBN triflate,9-borabicyclo[3.3.1]nonan-9-yl trifluoromethanesulfonate

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 : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P201 Obtain special instructions before use.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P273 Avoid release to the environment.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P308+P313 IF exposed or concerned: Get medical advice/attention.
P331 Do NOT induce vomiting.

Hazard statements

H225 Highly Flammable liquid and vapour
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H336 May cause drowsiness or dizziness
H373 May cause damage to organs through prolonged or repeated exposure
H411 Toxic to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

Product name : 9-BBN triflate
Synonyms : 9-BBN triflate,9-borabicyclo[3.3.1]nonan-9-yl trifluoromethanesulfonate

CAS : 62731-43-5
MF : C9H14BF3O3S
MW : 270.07

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. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

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

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

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.

Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

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. Risk of explosion.

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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Handle and store under inert gas. Air and moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

[Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['n-Hexane', '110-54-3', 'PC-TWA', '100 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical	['', 'Remarks', 'Skin', None, None]	['', 'Skin', None,	[Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['3- methylpentane', '96-14-0', 'TWA', '200 ppm', 'USA. ACGIH Threshold Limit Values (TLV)']	['', 'Remarks', 'Confirmed animal carcinogen with unknown relevance to humans',	['', 'TWA', '100 ppm350 mg/m3', 'USA. NIOSH Recommended Exposure Limits']	['', 'C', '510 ppm1,800 mg/m3', 'USA. NIOSH Recommended Exposure Limits']	['', 'PEL', '500 ppm1,800 mg/m3', 'California permissible exposure limits for chemical contaminants	['', 'STEL', '1,000 ppm3,600 mg/m3', 'California permissible exposure limits for chemical contaminants

	hazardous agents.].		hazardous agents.].				None, None]			(Title 8, Article 107)]	(Title 8, Article 107)]
--	---------------------	--	---------------------	--	--	--	-------------	--	--	-------------------------	-------------------------

Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis']	['n-Hexane', '110-54-3', '2,5- hexanedion e', '35micro mol per litre', 'Urine', 'China. Biological Occupational Exposure Indices']	['', 'Remarks', 'After shift', 'None, None, None]	['', '2,5- hexanedion e', '4 mg/l', 'Urine', 'China. Biological Occupational Exposure Indices']	['', 'After shift', 'None, None]
---	--	---	---	----------------------------------

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). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols 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. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	265.7±50.0 °C(Predicted)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	-22 °C
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	0.733 g/mL at 25 °C
Relative density	0.733 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.

t) Oxidizing properties	none
Solubility	sol common inert organic solvents such as Et ₂ O, CH ₂ Cl ₂ , and hexane.

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

Warming.

10.4 Incompatible materials

Oxidizing agents, Strong oxidizing agents

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture Acute toxicity

Oral: No data available

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: No data available

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

Remarks: No data available

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Remarks: No data available

Mixture causes damage to organs through prolonged or repeated exposure.

- Nervous system

Aspiration hazard

Classified based on available data. For more details, see section 2
Aspiration hazard, Aspiration may cause pulmonary edema and
pneumonitis.

11.2 Additional Information

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and
edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing,
laryngitis, Shortness of breath, Headache, Nausea

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components n-Hexane

Acute toxicity

LD50 Oral - Rat - male and female - 16,000 mg/kg (OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 172 mg/l - vapor

Remarks: (RTECS)

LD50 Dermal - Rabbit - male - > 2,000 mg/kg (OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 24 h (OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h (OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative (OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 478

Species: Mouse - male

Result: negative

Method: OECD Test Guideline 475

Species: Rat - male and female - Bone marrow

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

Inhalation - Causes damage to organs through prolonged or repeated exposure.

- Nervous system

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

3-methylpentane Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals.

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

May be fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

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

Components n-Hexane

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 2.5 mg/l - 96 h

Remarks: (ECOTOX Database)

Toxicity to daphnia EC50 - Daphnia magna (Water flea) - 2.1 mg/l - 48 h and other aquatic Remarks: (Lit.) invertebrates

3-methylpentane

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1208

IMDG: 1208

IATA-DGR: 1208

14.2 UN proper shipping name

ADR/RID: HEXANES,SOLUTION

IMDG: HEXANES,SOLUTION

IATA-DGR: Hexanes,SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA-DGR: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

Oxidizing agents, Strong oxidizing agents

SECTION 15: Regulatory information

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

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222222937

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.