

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.8

Revision Date 02.09.2024

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : 9-Borabicyclo[3.3.1]nonane solution

Product Number : 459496

Brand : Aldrich

REACH No. : This product is a mixture. REACH Registration Number see section 3.

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

Identified uses : Laboratory chemicals, Manufacture of substances

Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Substances and mixtures which in contact with water emit flammable gases, (Category 1)	H260: In contact with water releases flammable gases which may ignite spontaneously.
Skin irritation, (Category 2)	H315: Causes skin irritation.
Eye irritation, (Category 2)	H319: Causes serious eye irritation.
Reproductive toxicity, (Category 2)	H361f: Suspected of damaging fertility.
Specific target organ toxicity -	H336: May cause drowsiness or dizziness.

single exposure, (Category 3),
Central nervous system

Specific target organ toxicity -
repeated exposure, (Category 1),
Nervous system

H372: Causes damage to organs through
prolonged or repeated exposure if inhaled.

Aspiration hazard, (Category 1)

H304: May be fatal if swallowed and enters
airways.

Long-term (chronic) aquatic
hazard, (Category 2)

H411: Toxic to aquatic life with long lasting
effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word

Danger

Hazard Statements

H260

In contact with water releases flammable gases which may
ignite spontaneously.

H304

May be fatal if swallowed and enters airways.

H315

Causes skin irritation.

H319

Causes serious eye irritation.

H336

May cause drowsiness or dizziness.

H361f

Suspected of damaging fertility.

H372

Causes damage to organs (Nervous system) through prolonged
or repeated exposure if inhaled.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P231 + P232

Handle and store contents under inert gas. Protect from
moisture.

P273

Avoid release to the environment.

P301 + P310

IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

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.

P331

Do NOT induce vomiting.

Supplemental Hazard
Statements

none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word

Danger

Hazard Statements

H372

Causes damage to organs through prolonged or repeated
exposure if inhaled.

H304

May be fatal if swallowed and enters airways.

H361f	Suspected of damaging fertility.
Precautionary Statements	
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

2.3 Other hazards

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.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : 9-BBN

Formula : C₈H₁₅B

Molecular weight : 122,02 g/mol

Component		Classification	Concentration
n-Hexane			
CAS-No.	110-54-3	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 1; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H361f, H336, H372, H304, H411 Concentration limits: >= 5 %: STOT RE 2, H373; >= 20 %: STOT SE 3, H336;	>= 70 - < 90 %
EC-No.	203-777-6		
Index-No.	601-037-00-0		
Registration number	01-2119480412-44-XXXX		
3-methylpentane			
CAS-No.	96-14-0	Flam. Liq. 2; Skin Irrit. 2; Eye Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Chronic 2; H225, H315, H319, H336, H304, H411	>= 10 - < 20 %
EC-No.	202-481-4		
Index-No.	601-007-00-7 *		

*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, or the annual tonnage does not require a registration.

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 2.2) and/or in section 11

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

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Water Foam

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Borane/boron oxides

Combustible.

May not get in touch with: Water

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

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.

5.4 Further information

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. 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. Keep workplace dry. Do not allow product to come into contact with water.

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

Tightly closed. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.
Never allow product to get in contact with water during storage.

Handle and open container with care. Handle and store under inert gas.

Storage class

Storage class (TRGS 510): 4.3: Hazardous materials, which set free flammable gases upon contact with water

7.3 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

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

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

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.

Recommended Filter type: Filter type ABEK

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.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical 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 | 68 - 70 °C |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | No data available |
| h) Flash point | Not applicable |
| 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 | 0,691 g/mL at 25 °C |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| | |
| s) Explosive properties | Not classified as explosive. |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Moisture.

10.5 Incompatible materials

Oxidizing agents, Strong oxidizing agents

10.6 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

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Evidence to impair 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

No data available Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Warning: contains n-hexane (CAS#110-54-3) a suspected neurotoxin.

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

No data available

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

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

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

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.

12.6 Endocrine disrupting properties

Product:

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission

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)
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Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 2,1 mg/l - 48 h Remarks: (Lit.)
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3-methylpentane

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3399

IMDG: 3399

IATA: 3399

14.2 UN proper shipping name

ADR/RID: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (n-Hexane, methylcyclopentane, 9-Borabicyclo[3.3.1]nonane) (n-Hexane, methylcyclopentane, 9-Borabicyclo[3.3.1]nonane)

IMDG: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (n-Hexane, 9-Borabicyclo[3.3.1]nonane, methylcyclopentane) (n-Hexane, 9-Borabicyclo[3.3.1]nonane, methylcyclopentane)

IATA: Organometallic substance, liquid, water-reactive, flammable (n-Hexane, 9-Borabicyclo[3.3.1]nonane, methylcyclopentane) (n-Hexane, 9-Borabicyclo[3.3.1]nonane, methylcyclopentane)

Passenger Aircraft: Not permitted for transport

14.3 Transport hazard class(es)

ADR/RID: 4.3 (3)

IMDG: 4.3 (3)

IATA: 4.3 (3)

14.4 Packaging group

ADR/RID: I

IMDG: I

IATA: I

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (B/E)

Further information : No data available

SECTION 15: Regulatory information

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

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

Authorisations and/or restrictions on use

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

E2

ENVIRONMENTAL HAZARDS

O2

OTHER HAZARDS

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H225	Highly flammable liquid and vapor.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
H361f	Suspected of damaging fertility.
H372	Causes damage to organs through prolonged or repeated exposure if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.
H411	Toxic to aquatic life with long lasting effects.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

Classification of the mixture

Water-react1	H260
Skin Irrit.2	H315
Eye Irrit.2	H319
Repr.2	H361f
STOT SE3	H336
STOT RE1	H372
Asp. Tox.1	H304
Aquatic Chronic2	H411

Classification procedure:

Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method
Calculation method

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact

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