

MATERIAL SAFETY DATA SHEET (MSDS)

according to Regulation (EC) No. 1907/2006

Version 3.0 Revision Date 03.07.2017


1.0 Identification of the substance/preparation and of the company/enterprise

- 1.1 Product identifiers** (-)-Diisopinocampheylchloroborane in heptane, 50-65 % w. solution
EINECS : not listed
CAS : 85116-37-6
RTECS : not listed
- 1.2 Relevant identified uses of the substance or mixture and uses advised against**
 Enantioselective reducing agent
- 1.3 Details of the supplier of the safety data sheet**
 JSC AVIABOR, Nizhny Novgorod Region
 606000 Dzerzhinsk, Russia
 Tel: (+7)-8313-249 727, Fax: (+7)-8313-249 767
 Only Representative – Espace Chemicals GmbH
 Tel.: +49(0) 30 896779290 – 0, Fax: + 49(0) 30 896779290 – 1
- 1.4 Emergency telephone number:** (+7)-8313-249 750/630

2.0 Hazards Identification

2.1 Classification of the substance or mixture

Regulation (EC) No 1272/2008 Annex VI Table

Classification		Labelling		
Hazard Class and Category Code(s)	Hazard Statement Code(s)	Pictogram Signal Word Code(s)	Hazard Statement Code(s)	Suppl. Hazard Statement Code(s)
Flam. Liq. 2 Skin Corr. 1B STOT SE. 3 Asp. Tox. 1 Aquatic Acute. 1 Aquatic Chronic. 1	H225 H314 H336 H304 H400 H410	 Danger	H225 H314 H336 H304 H400 H410	-

2.2 Label elements

Hazard Statement

- H225 Highly flammable liquid and vapour.
 H314 Causes severe skin burns and eye damage.
 H336 May cause drowsiness or dizziness.
 H304 May be fatal if swallowed and enters airways.
 H400 Very toxic to aquatic life.
 H410 Toxic to aquatic life.

Precautionary statement(s)

- P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.
 P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
 P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

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.

3.0 Composition/Information on Ingredients

3.2 Mixture

(-)-Diisopinocampheylchloroborane

Concentration	50-65 wt%
CAS-No.	85116-37-6
EINECS	not listed
Chemical formula:	C ₂₀ H ₃₄ BCl
Molar mass	320.76
IUPAC Name	Chlorobis[(1R,2S,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]hept-3-yl]borane
Classification:	Flam. Liq. 2; Met. Corr. 1; Skin Corr. 1B; STOT RE. 2; H225, H290, H314, H373

Heptane

Concentration	20-35 wt%
CAS-No.	142-82-5
EINECS	205-563-8
Chemical formula:	C ₇ H ₁₆
Molar mass	100.20
Classification:	Flam. Liq.2; Skin Irrit.2; STOT SE3; Asp. Tox.1; Aquatic Acute1; Aquatic Chronic 1; H225, H304, H315, H336, H400, H410

α-Pinene

Concentration	~15 wt%
CAS-No.	80-56-8
EINECS	201-291-9
Chemical formula:	C ₁₀ H ₁₆
Molar mass	136.24
IUPAC Name	2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene
Classification:	Flam. Liq.3; Skin Irrit.2; Skin Sens.1; Asp. Tox.1; H226, H304, H315, H317

4.0 First Aid Measures

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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.

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

5.0 Fire Fighting Measures

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides, hydrogen chloride gas, borane/boron oxides.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6.0 Accidental Release Measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas. For personal protection see section 8.

6.2 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.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing, and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7.0 Handling and Storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Hydrolyses readily. Handle and store under inert gas. Light sensitive. Moisture sensitive.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

8.0 Exposure Control / Personal Protection

8.1 Control parameters

Components with workplace control parameters

8.2 Exposure controls

Engineering controls

Safety shower and eye bath. Use only in a chemical fume hood.

General hygiene measures

During processing ensure efficient exhaust ventilation in the working area. Wash hands before breaks of the work and after working with the substance. Keep working clothes separate. Wash thoroughly after handling. Wash contaminated clothing before reuse. Discard contaminated shoes.

Personal protective equipment

Respiratory Protection	: breathing mask
Hand Protection	: rubber gloves
Eye Protection	: closely fitting goggles
Skin Protection	: protective clothing

9.0 Physical and Chemical Properties

9.1 Information on basic physical and chemical properties

Form	: liquid
Colour	: colourless to slightly yellow
Odour	: strong pinene odour
pH	: decomposition by water
BP/BP Range	: N/A for mixture; 98 °C for heptane, 156 °C for α -pinene
MP/MP Range	: N/A
Flash Point	: - 2 °C for mixture; -4 °C for heptane, 33 °C for α -pinene
Flammability	: N/A
Autoignition Temp.	: 227 °C for mixture; 257 °C for heptane, 255 °C for α -pinene
Oxidizing Properties	: N/A
Explosive Properties	: N/A
Explosion Limits Lower	: N/A
Vapour Pressure	: 48 hPa at 20 °C for heptane, 5 hPa at 25 °C for α -pinene
SG/Density	: 0.90-0.92 g/ml
Partition Coefficient	: N/A
Viscosity	: N/A
Vapour Density	: N/A
Saturated Vapour Conc.	: N/A
Evaporation Rate	: N/A
Bulk Density	: N/A
Decomposition Temp.	: N/A
Solvent Content	: 20-35 wt% heptane and 15 wt% α -pinene
Water Content	: N/A
Surface Tension	: N/A
Conductivity	: N/A
Miscellaneous Data	: N/A
Solubility	: N/A

9.2 Other safety information

Stability to air : (-)-Diisopinocampheylchloroborane is a hygroscopic material, in moist air it will hydrolyze releasing hydrogen chloride gas.

10.0 Stability and Reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

Stable.

10.3 Possibility of hazardous reactions

Develops hydrochloric acid on contact with water.

10.4 Conditions to avoid

Stable. Keep away from heat, sparks, and flame.

10.5 Incompatible materials

Water, air, acids, alcohols, oxidizing agents.

10.6 Hazardous decomposition products

Carbon dioxide, boron oxides, hydrogen chloride.

11.0 Toxicological Information

11.1 Information on toxicological effects

Acute toxicity

No information found for the product.

Heptane is a skin irritant and a central nervous system depressant. Inhalation may cause laboured breathing, dullness, drowsiness, confusion, coughing, respiratory tract irritation, light headedness, incoordination, loss of appetite, giddiness, and hallucinations. Repeated or prolonged exposure may cause central nervous system depression and unconsciousness. Skin contact may cause redness, irritation, pain, and defatting dermatitis.

Repeated or prolonged contact may cause dermatitis. Eye contact may cause redness, pain, visual disturbances, and conjunctivitis.

Heptane can be aspirated into the lungs with the risk of pulmonary edema, hemorrhage, and pneumonia.

TCLo (inhalation-human) : 1000 pph/6 minutes, CNS effects

For α -pinene, LD₅₀ (oral-rat) : 700 mg/kg

LC₅₀ (inhalation-rat) : 625 mg/m³

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

Eyes: no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

IARC: No component of this product presents at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Potential health effects

Inhalation May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract. Vapours may cause drowsiness and dizziness.

Ingestion May be harmful if swallowed. Causes burns. Aspiration hazard if swallowed – can enter lungs and cause damage.

Skin May be harmful if absorbed through skin. Causes skin burns.

Eyes Causes eye burns.

Signs and Symptoms of Exposure

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.

Additional Information

RTECS: Not available

12.0 Ecological Information

12.1 Toxicity

No environmental toxicity data for the product.

For n-heptane: EC₅₀ *Daphnia magna* (Water flea) – 1.50 mg/l/48 hr.

LC₅₀ *Carassius auratus* (Goldfish) - 4 mg/l/24 hr.

12.2 Persistence and degradability : NDA

12.3 Bioaccumulative potential : NDA

12.4 Mobility in soil : NDA

12.5 Results of PBT and vPvB assessment : NDA

12.6 Other adverse effects

Extensive monitoring data indicates n-heptane is a widely occurring atmospheric pollutant.

Photolysis and hydrolysis of n-heptane are not expected to be important in soils or in aquatic environments. The biodegradation of n-heptane may occur in soils and aquatic environments; however, volatilization and adsorption are expected to be far more important fate processes.

α -Pinene is expected to biodegrade under aerobic conditions if released to the soil and if released in both fresh and salt water systems.

13.0 Disposal Consideration

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14.0 Transport Information

14.1 UN-Number

2924

14.2 UN proper shipping name

Flammable liquid, corrosive, n.o.s. ((-)-Diisopinocampheylchloroborane, in heptane, α -pinene)

14.3 Transport hazard class(es)

GGVS/GGVE/ADR/RID: 3, Hazard Identification: 338, Classification: FC, Tunnel Code: (C/E)

IMO/GGVSee: 3 (Sub.8), MFAG: 760, EmS: F-E, S-C, Stowage: E

ICAO/IATA: 3 (Sub.8), PAX: 350, CAO: 360, Limited quantity: F

14.4 Packaging group

GGVS/GGVE/ADR/RID: I IMO/GGVSee: I ICAO/IATA: I

14.5 Environmental hazards

GGVS/GGVE/ADR/RID: No IMO/GGVSee: "MARINE POLLUTANT" ICAO/IATA: No

14.6 Special precautions for user

See section 7.0

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

The substance is not intended to be transported in bulk.

15.0 Regulatory Information

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

no data available

15.2 Chemical Safety Assessment

no data available

16.0 Other Information

This material safety data sheet was prepared in compliance with laws, regulations and administrative provisions relative to classification, packaging and labelling of dangerous substances and preparations.

This information is to the best of Aviabor's current knowledge and is intended to describe the product only in terms of health and safety and environmental requirements. Since the conditions of use are outside our control, any recommendations or suggestions are made without guarantee and we disclaim any liability for loss or damage suffered from use of this information. Customers must satisfy themselves that the product is suitable for a particular purpose. Furthermore, nothing contained herein shall be construed as a recommendation to use any product in conflict with existing patents.