

**MATERIAL SAFETY DATA SHEET (MSDS)  
according to Regulation (EC) No. 1907/2006  
Version 2.1 Revision Date 23.06.2017**

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

- 1.1 Product identifiers** : (S)-Methyl-oxazaborolidine, 1 M solution in toluene  
**EINECS** : 601-150-5  
**CAS** : 112022-81-8  
**RTECS** : not listed
- 1.2 Relevant identified uses of the substance or mixture and uses advised against**  
 Catalyst for enantioselective reduction of ketones.
- 1.3 Details of the supplier of the safety data sheet**  
 JSC AVIABOR, Nizhny Novgorod Region  
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 Tel: (+7)-8313-249 727, Fax: (+7)-8313-249 767  
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- 1.4 Emergency telephone number** (+7)-8313-249 750/ 630

## 2.0 Hazards Identification

- 2.1 Classification of the substance or mixture**  
 Highly flammable. Irritating to skin. Harmful: danger of serious damage to health by prolonged Exposure through inhalation. Possible risk of harm to the unborn child. Harmful: may cause lung damage if swallowed. Vapours may cause drowsiness and dizziness.
- 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	H225		H225	-
Acute Tox. Oral. 4	H302		H302	
Eye Dam. 1	H318		H318	
Skin Irrit. 2	H315		H315	
STOT RE 2	H373		H373	
Repr. 2	H361d		H361d	
Asp.Tox. 1	H304		H304	
STOT SE 3	H336	H336		
		Danger		

## 2.2 Label elements

**Hazard statement(s):**

- H225 Highly flammable liquid and vapour.  
 H302 Harmful if swallowed.  
 H318 Causes serious eye damage.  
 H315 Causes skin irritation.  
 H373 May cause damage to organs through prolonged or repeated exposure.  
 H361d Suspected of damaging the unborn child.  
 H304 May be fatal if swallowed and enters airways.  
 H336 May cause drowsiness or dizziness.

**Precautionary statement(s)**

P210	Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P264	Wash hands thoroughly after handling.
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P271	Use only outdoors or in a well-ventilated area.
P201	Obtain special instructions before use.
P331	Do NOT induce vomiting.
P308+P313	IF exposed or concerned: Get medical advice/attention.
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P405	Store locked up.

**3.0 Composition / Information on Ingredients**

Trade names/Synonyms	(S)-Methyl-oxazaborolidine; (S)-3,3-Diphenyl-1-methyltetrahydro-3H-pyrrolo[1,2-c][1,3,2]oxazaborole; (S)-2-Methyl-CBS-oxazaborolidine; (S)-3,3-Diphenyl-1-methylpyrrolidino[1,2-c]-1,3,2-oxazaborole
Compound	(S)-Methyl-oxazaborolidine
Contents	27-33 wt%
Chemical formula	C <sub>18</sub> H <sub>20</sub> BNO
CAS-No.	112022-81-8
EINECS	601-150-5
Molar mass	277.18 g/mol
R & S-Phrases:	R 11, 22, 38, 41, 48/20, 63, 65, 67 S 2, 36/37, 46, 62
Compound	Toluene
Contents	67-73 wt%
Chemical formula	C <sub>7</sub> H <sub>8</sub>
CAS-No.	108-88-3
EINECS	203-625-9
Molar mass	92.14 g/mol
Classification	Flam. Liq. 2; Repr. 2; Asp. Tox. 1; STOT RE 2; Skin Irrit. 2; STOT SE 3; H225, H304, H315, H336, H361d, H373

**4.0 First Aid Measures****4.1 Description of first aid measures****After skin contact**

Immediately wash skin with soap and plenty of water while removing contaminated clothing and shoes. Call a doctor.

**After eyes contact**

Immediately flush eyes with plenty of water for at least 20 minutes while holding eyelids open. Call a doctor.

**After ingestion**

If swallowed wash out mouth with water provided person is conscious. Call a doctor.

**After inhalation**

Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

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

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

**4.3 Indication of immediate medical attention and special treatment needed**

no data available

**5.0 Fire Fighting Measures****5.1 Extinguishing media**

**Suitable extinguishing media**

Carbon dioxide, dry chemical powder.

**Unsuitable extinguishing media**

Do not use water (toluene will float on water).

**5.2 Special hazards arising from the substance or mixture**

Nature of decomposition products not known.

**5.3 Precautions for fire-fighters**

Wear self-contained breathing apparatus for fire fighting if necessary.

**5.4 Further information - no data available****6.0 Accidental Release Measures****6.1 Personal precautions, protective equipment and emergency procedures**

Wear recommended personal protective equipment. Eliminate ignition sources.

**6.2 Environmental precautions**

Do not allow to enter sewerage system.

**6.3 Methods and materials for containment and cleaning up**

Mix with large amounts of dry inert absorbent material such as soda ash or sand. Using non-sparking tools, scoop solids into a dry metal container, properly label and cover. Take immediately to a waste handling area. Properly dispose of all residues immediately.

Handle in compliance with all local, state, and federal laws and regulations.

**6.4 Reference to other sections**

For disposal see section 13.

**7.0 Handling and Storage****7.1 Precautions for safe handling**

Eating, drinking, smoking as well as keeping of foods in a workroom forbidden. Take precautionary measures against static discharges. Do not expose to air. Handle and store in a closed system under dry nitrogen gas. Use non-sparking tools when opening or closing containers.

**7.2 Conditions for safe storage, including any incompatibilities**

Store under dry nitrogen gas in a dry, well-ventilated place. Do not store with oxidizing substances. Keep tightly closed. Keep away from heat, sparks, and open flame.

**7.3 Specific end uses**

no data available

**8.0 Exposure Controls / Personal Protection****8.1 Control parameters****Components with workplace control parameters****8.2 Exposure controls****Engineering controls**

Safety shower and eye bath. During processing ensure efficient exhaust ventilation in the working area.

**General hygiene measures**

Wash contaminated clothing before reuse. Wash thoroughly after handling.

**Personal protective equipment**

Respiratory Protection : Government approved respirator.

Hand Protection : Compatible chemical-resistant gloves.

Eye Protection : Chemical safety goggles.

Skin Protection : Protective clothing.

Special Protective Measures : Face shield.

**9.0 Physical and Chemical Properties****9.1 Information on basic physical and chemical properties**

Form : Liquid

Colour : Colourless to yellow

pH : N/A

BP/BP Range : 111 °C for toluene

MP/MP Range : N/A

Flash Point : 4 °C for toluene

Flammability	: N/A	Autoignition Temp	: 460 °C for toluene
Oxidizing Properties	: N/A	Explosive Properties	: N/A
Explosion Limits Lower	: N/A	Vapor Pressure	: N/A
SG/Density	: 0.92-0.95	Partition Coefficient	: N/A
Viscosity	: N/A	Vapor Density	: N/A
Saturated Vapor Conc.	: N/A	Evaporation Rate	: N/A
Bulk Density	: N/A	Decomposition Temp.	: N/A
Solvent Content	: N/A	Water Content	: N/A
Surface Tension	: N/A	Conductivity	: N/A
Miscellaneous Data	: N/A	Solubility in water	: N/A

## 10.0 Stability and Reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

Reacts with water.

### 10.4 Conditions to avoid

Stable. Keep away from heat, sparks, and flame. Store under dry nitrogen. Decompose on exposure to moist air or water.

### 10.5 Incompatible materials

Oxidizing agents. Reacts with water.

### 10.6 Hazardous decomposition products

Boron oxides, nitrogen oxides, carbon dioxide, carbon monoxide.

## 11.0 Toxicological Information

### 11.1 Information on toxicological effects

#### Acute toxicity

No information found for the product.

LD<sub>50</sub> (oral-rat): estimated 300-500 mg/kg for (S)-methyl oxazaborolidine

LD<sub>50</sub> (oral-rat): 636 mg/kg for toluene,

LC<sub>50</sub> (inhalation-rat): 49 g/m<sup>3</sup> for toluene,

LD<sub>50</sub> (skin-rabbit): 14100 ml/kg for toluene.

#### Irritation and corrosion

no data available

#### Sensitisation

no data available

#### Chronic exposure

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Toluene)

#### Signs and Symptoms of Exposure

Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the penis, prepuce, and scrotum in animals.

#### Potential Health Effects

**Inhalation** Harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.

**Skin** May be harmful if absorbed through skin. Causes skin irritation.

**Eyes** May cause eye irritation.

**Ingestion** May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

**Target Organs** Bladder, liver, kidney, brain.

## 12.0 Ecological Information

12.1 Toxicity : 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** : no data available  
 12.6 **Other adverse effects** : no data available

### 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

1294

#### 14.2 UN proper shipping name

Toluene

#### 14.3 Transport hazard class(es)

GGVS/GGVE/ADR/RID: 3, Hazard Identification: 33, Classification: F1, Tunnel Code: (D/E)

IMO/GGVSee: 3, MFAG: 310, EmS: F-E, S-D, Stowage cat. B

ICAO/IATA: 3, PAX: 654, CAO: 662

#### 14.4 Packaging group

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

#### 14.5 Environmental hazards

GGVS/GGVE/ADR/RID: No      IMO/GGVSee: No      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.

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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.