

SAFETY DATA SHEET

Version 8.11
Revision Date 03/02/2024
Print Date 06/08/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : (S)-(-)-2-Methyl-CBS-oxazaborolidine
solutionProduct Number : 457701
Brand : Aldrich**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +1 314 771-5765
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318

Aldrich - 457701

Page 1 of 14

Reproductive toxicity (Category 2), H361
 Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
 Specific target organ toxicity - repeated exposure (Category 2), Central nervous system, H373
 Aspiration hazard (Category 1), H304
 Short-term (acute) aquatic hazard (Category 2), H401
 Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H373	May cause damage to organs (Central nervous system) through prolonged or repeated exposure.
H401	Toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
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/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338 +	IF IN EYES: Rinse cautiously with water for several minutes.

P310	Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms	: (S)-Tetrahydro-1-methyl-3,3-diphenyl-1H,3H-pyrrolo[1,2-c][1,3,2]oxazaborole (S)-3,3-Diphenyl-1-methyltetrahydro-3H-pyrrolo[1,2-c][1,3,2]oxazaborole α,α -Diphenyl-L-prolinol methylboronic acid cycl-amide ester (S)-1-Methyl-3,3-diphenyl-tetrahydro-pyrrolo[1,2c][1,3,2]oxazaborole
Formula	: C ₁₈ H ₂₀ BNO
Molecular weight	: 277.17 g/mol

Component	Classification	Concentration
Toluene		
CAS-No. 108-88-3 EC-No. 203-625-9 Index-No. 601-021-00-3 Registration number 01-2119471310-51-XXXX	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H315, H361, H336, H373, H304, H401, H412 Concentration limits: 20 %: STOT SE 3, H336;	>= 90 - <= 100 %
(S)-methyl oxazaborolidine		
CAS-No. 112022-81-8	Acute Tox. 4; Eye Dam. 1; H302, H318	>= 30 - < 50 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

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

In case of skin contact

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NO_x)
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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors 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 non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

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

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

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.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

Component	CAS-No.	Value	Control parameters	Basis
Toluene	108-88-3	TWA	100 ppm 375 mg/m ³	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		STEL	150 ppm 560 mg/m ³	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)
		TWA	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
	Remarks	Z37.12-1967		
		CEIL	300 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		Peak	500 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Visual impairment Female reproductive Pregnancy loss 2023 Adoption Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		TWA	100 ppm 375 mg/m ³	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 560 mg/m ³	USA. NIOSH Recommended Exposure Limits

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Toluene	108-88-3	Toluene	0.02 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	Prior to last shift of workweek			
		Toluene	0.03 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

		o-Cresol	0.3mg/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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

9.1 Information on basic physical and chemical properties

- | | |
|---------------------------------|----------------------------|
| a) Appearance | Form: liquid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point | 111 °C 232 °F at 1,013 hPa |

Aldrich - 457701

Page 7 of 14

- and boiling range
- g) Flash point 4 °C (39 °F) - closed cup
 - h) Evaporation rate No data available
 - i) Flammability (solid, gas) No data available
 - j) Upper/lower flammability or explosive limits No data available
 - k) Vapor pressure No data available
 - l) Vapor density No data available
 - m) Density 0.929 g/cm³
Relative density No data available
 - n) Water solubility No data available
 - o) Partition coefficient: n-octanol/water No data available
 - p) Autoignition temperature No data available
 - q) Decomposition temperature No data available
 - r) Viscosity 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

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

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

Acute toxicity estimate Oral - 1,667 mg/kg
(Calculation method)

Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - 25.7 mg/l - vapor(Calculation method)

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

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.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

11.2 Additional Information

Lung irritation, chest pain, pulmonary edema, Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the penis, prepuce, and scrotum in animals.

Aldrich - 457701

Page 9 of 14

Components

Toluene

Acute toxicity

LD50 Oral - Rat - male - 5,580 mg/kg
(Directive 67/548/EEC, Annex V, B.1.)
LC50 Inhalation - Rat - male - 4 h - 25.7 mg/l - vapor
(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male - > 5,000 mg/kg
Remarks: (ECHA)

Skin corrosion/irritation

Skin - Rabbit
Result: irritating - 4 h
(Regulation (EC) No. 440/2008, Annex, B.4)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig
Result: negative
(Regulation (EC) No. 440/2008, Annex, B.6)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Result: negative
Test Type: Ames test
Test system: S. typhimurium
Result: negative
Species: Rat - Bone marrow
Result: negative
Remarks: (ECHA)

Carcinogenicity

No data available

Reproductive toxicity

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

Inhalation - 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 - May cause damage to organs through prolonged or repeated exposure.
- Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

Aspiration may cause pulmonary edema and pneumonitis.

(S)-methyl oxazaborolidine**Acute toxicity**

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

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

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

Components

Toluene

Toxicity to fish	flow-through test LC50 - Oncorhynchus kisutch (coho salmon) - 5.5 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Ceriodaphnia dubia (water flea) - 3.78 mg/l - 48 h (US-EPA)
Toxicity to bacteria	static test EC50 - Bacteria - 84 mg/l - 24 h Remarks: (ECHA)
Toxicity to fish(Chronic toxicity)	flow-through test NOEC - Oncorhynchus kisutch (coho salmon) - 1.39 mg/l - 40 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	NOEC - Ceriodaphnia dubia (water flea) - 0.74 mg/l - 7 d (US-EPA)

(S)-methyl oxazaborolidine

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

Aldrich - 457701

Page 12 of 14

SECTION 14: Transport information**DOT (US)**

UN number: 1294 Class: 3 Packing group: II
Proper shipping name: TolueneSOLUTION

Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1294 Class: 3 Packing group: II EMS-No: F-
E, S-D
Proper shipping name: TOLUENESOLUTION

IATA

UN number: 1294 Class: 3 Packing group: II
Proper shipping name: TolueneSOLUTION

SECTION 15: Regulatory information**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

(S)-methyl oxazaborolidine 112022-81-8

Toluene CAS-No. 108-88-3 Revision Date 2007-07-01

New Jersey Right To Know Components

Toluene CAS-No. 108-88-3 Revision Date 2007-07-01

(S)-methyl oxazaborolidine 112022-81-8

California Prop. 65 Components

, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov. Toluene CAS-No. 108-88-3 Revision Date 2009-02-01

SECTION 16: Other information

Further information

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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 with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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