

**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : 4-Methylpyridine-2-boronic acid *N*-phenyldiethanolamine ester

Product Number : 648841

Brand : Aldrich

CAS-No. : 849100-03-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable solids (Category 1), H228

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

Skin sensitisation (Category 1), H317

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 statement(s)

H228

Flammable solid.

H315

Causes skin irritation.

H317

May cause an allergic skin reaction.

H318

Causes serious eye damage.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P261

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

P264

Wash skin thoroughly after handling.

P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/doctor.
P333 + P313	If skin irritation or rash 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.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.2 Mixtures

Synonyms	:	4-Methyl-2-pyridineboronic acid N-phenyldiethanolamine ester 4-Methyl-2-pyridineboronic acid[2,2 $\phi$ -(phenylimino)diethanol]ester
Formula	:	C <sub>16</sub> H <sub>19</sub> BN <sub>2</sub> O <sub>2</sub>
Molecular weight	:	282.15 g/mol

#### Hazardous components

Component	Classification	Concentration
<b>2-Propanol</b>		
CAS-No.	67-63-0	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336
EC-No.	200-661-7	
Index-No.	603-117-00-0	
Registration number	01-2119457558-25-XXXX	
<b>2,2'-Phenyliminodiethanol</b>		
CAS-No.	120-07-0	Eye Dam. 1; Aquatic Acute 3; Aquatic Chronic 3; H318, H412
EC-No.	204-368-5	
<b>Lithium bromide</b>		
CAS-No.	7550-35-8	Skin Irrit. 2; Eye Irrit. 2A; Skin Sens. 1; H315, H317, H319
EC-No.	231-439-8	

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

## 4. 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. 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

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### 5. FIREFIGHTING 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

No data available

#### 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.

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### 6. ACCIDENTAL RELEASE MEASURES

#### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Avoid breathing dust. 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.

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

Sweep up and shovel. 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). Keep in suitable, closed containers for disposal. Contain spillage, pick up with an electrically protected vacuum cleaner or by wet-brushing and transfer to a container for disposal according to local regulations (see section 13).

#### 6.4 Reference to other sections

For disposal see section 13.

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### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed. 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

Keep container tightly closed in a dry and well-ventilated place.

Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

#### 7.3 Specific end use(s)

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

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### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
2-Propanol	67-63-0	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		STEL	400 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		
		TWA	400 ppm 980 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	500 ppm 1,225 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	400 ppm 980 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		PEL	400 ppm 980 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	500 ppm 1,225 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Hazardous components without workplace control parameters

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
alcohol	-	Acetone	40 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			

## 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

Face shield and safety glasses 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 particle respirator type N100 (US) or type P3 (EN 143) 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: solid  |
| b) Odour  | No data available  |
| c) Odour Threshold                              | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | Melting point/range: 267 - 271 °C (513 - 520 °F) - dec.            |
| f) Initial boiling point and boiling range      | No data available  |
| g) Flash point                                  | No data available  |
| h) Evaporation rate                             | No data available  |
| i) Flammability (solid, gas)                    | The substance or mixture is a flammable solid with the category 1. |
| j) Upper/lower flammability or explosive limits | No data available  |
| k) Vapour pressure                              | No data available  |
| l) Vapour density                               | No data available  |
| m) Relative density                             | No data available  |
| n) Water solubility                             | No data available  |
| o) Partition coefficient: n-octanol/water       | No data available  |
| p) Auto-ignition temperature                    | No data available  |
| q) Decomposition temperature                    | No data available  |
| r) Viscosity                                    | No data available  |
| s) Explosive properties                         | No data available  |
| t) Oxidizing properties                         | No data available  |

### 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Reacts with air to form peroxides.  
Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

#### 10.4 Conditions to avoid

Heat, flames and sparks.

#### 10.5 Incompatible materials

No data available

#### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen bromide gas, Borane/boron oxides, Lithium oxides

Other decomposition products - No data available

In the event of fire: see section 5

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### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

Inhalation: No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

Dermal: No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Skin corrosion/irritation

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Serious eye damage/eye irritation

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Respiratory or skin sensitisation

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Germ cell mutagenicity

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Carcinogenicity

IARC: No component 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 component 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 (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Specific target organ toxicity - single exposure

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Specific target organ toxicity - repeated exposure

No data available

##### Aspiration hazard

No data available (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

##### Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

Kidney - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

Kidney - Irregularities - Based on Human Evidence (2-Propanol)

Stomach - Irregularities - Based on Human Evidence (Lithium bromide)

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## 12. 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 (4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester)

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

No data available

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## 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.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 3175      Class: 4.1      Packing group: II  
Proper shipping name: Solids containing flammable liquid, n.o.s. (2-Propanol)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 3175      Class: 4.1      Packing group: II      EMS-No: F-A, S-I  
Proper shipping name: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (2-Propanol)

### IATA

UN number: 3175      Class: 4.1      Packing group: II  
Proper shipping name: Solids containing flammable liquid, n.o.s. (2-Propanol)

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## 15. REGULATORY INFORMATION

### SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

### SARA 313 Components

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

	CAS-No.	Revision Date
2-Propanol	67-63-0	2007-03-01

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

### Massachusetts Right To Know Components

	CAS-No.	Revision Date
2-Propanol	67-63-0	2007-03-01

### Pennsylvania Right To Know Components

4-Methyl-2-Pyridineboronic Acid N-Phenyldiethanolamine Ester	CAS-No. 849100-03-4	Revision Date
2-Propanol	67-63-0	2007-03-01
2,2'-Phenyliminodiethanol	120-07-0	
Lithium bromide	7550-35-8	

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

**16. OTHER INFORMATION**

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Eye Dam.	Serious eye damage
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H228	Flammable solid.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
H412	Harmful to aquatic life with long lasting effects.
Skin Irrit.	Skin irritation
Skin Sens.	Skin sensitisation
STOT SE	Specific target organ toxicity - single exposure

Further information

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**Preparation Information**

Sigma-Aldrich Corporation  
 Product Safety – Americas Region  
 1-800-521-8956

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