

## SAFETY DATA SHEET

Version 6.1  
Revision Date 07/02/2019  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : (±)-Hydroxybupropion-D<sub>6</sub> solution

Product Number : H-062  
Brand : Cerilliant  
Index-No. : 608-001-00-3

**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 Inc.  
3050 Spruce Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887

**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  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Eye irritation (Category 2A), H319

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)  
H225 : Highly flammable liquid and vapour.  
H302 + H312 + H332 : Harmful if swallowed, in contact with skin or if inhaled.

|                            |  |
|----------------------------|--|
| H319                       | Causes serious eye irritation.   |
| Precautionary statement(s) |  |
| 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.  |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapours/ 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.  |
| P280                       | Wear protective gloves/ protective clothing/ eye protection/ face protection.  |
| P301 + P312 + P330         | IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.   |
| 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. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.   |
| P363                       | Wash contaminated clothing before reuse.   |
| P370 + P378                | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.   |
| P403 + P235                | Store in a well-ventilated place. Keep cool.   |
| 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

| Component           | Classification        | Concentration  |
|---------------------|-----------------------|--|
| <b>Acetonitrile</b> |                       |  |
| CAS-No.             | 75-05-8               | Flam. Liq. 2; Acute Tox. 4;<br>Eye Irrit. 2A; H225, H302,<br>H332, H312, H319<br><br>>= 90 - <=<br>100 % |
| EC-No.              | 200-835-2             |  |
| Index-No.           | 608-001-00-3          |  |
| Registration number | 01-2119471307-38-XXXX |  |
|                     |                       |  |

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

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## SECTION 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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## SECTION 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

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

### 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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## SECTION 6: 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.

### 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.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

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

Use explosion-proof equipment. 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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Recommended storage temperature -20 °C

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

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Components with workplace control parameters

| Component    | CAS-No. | Value  | Control parameters             | Basis   |
|--------------|---------|--|--------------------------------|---|
| Acetonitrile | 75-05-8 | TWA  | 20 ppm                         | USA. ACGIH Threshold Limit Values (TLV)   |
|              | Remarks | Lower Respiratory Tract irritation<br>Not classifiable as a human carcinogen<br>Danger of cutaneous absorption |                                |   |
|              |         | TWA  | 20 ppm<br>34 mg/m <sup>3</sup> | USA. NIOSH Recommended Exposure Limits  |
|              |         | Forms cyanide in the body.   |                                |   |
|              |         | TWA  | 40 ppm<br>70 mg/m <sup>3</sup> | USA. Occupational Exposure Limits (OSHA) - Table Z-1<br>Limits for Air Contaminants     |
|              |         | The value in mg/m <sup>3</sup> is approximate.   |                                |   |
|              |         | PEL  | 40 ppm<br>70 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|              |         | Skin   |                                |   |

|  |  |      |                                 |   |
|--|--|------|---------------------------------|---|
|  |  | STEL | 60 ppm<br>105 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|  |  | Skin |                                 |   |

## 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 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.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |  |                                      |
|--|--------------------------------------|
| a) Appearance                              | Form: liquid                         |
| b) Odour                                   | No data available                    |
| c) Odour Threshold                         | No data available                    |
| d) pH                                      | No data available                    |
| e) Melting point/freezing point            | No data available                    |
| f) Initial boiling point and boiling range | 81 - 82 °C 178 - 180 °F at 1.013 hPa |
| g) Flash point                             | 2 °C (36 °F) - closed cup            |
| h) Evaporation rate                        | No data available                    |

|   |   |
|---|---|
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V)<br>Lower explosion limit: 4.4 %(V) |
| k) Vapour pressure                              | No data available   |
| l) Vapour density                               | No data available   |
| m) Relative density                             | 0.782 g/cm <sup>3</sup> at 20 °C (68 °F)                          |
| 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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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

acids, Bases, Oxidizing agents, Alkali metals

### 10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### 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

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

#### Additional Information

RTECS: Not available

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

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis

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## SECTION 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

### 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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## SECTION 13: Disposal considerations

### 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. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

UN number: 1648 Class: 3 Packing group: II  
Proper shipping name: AcetonitrileSOLUTION

Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: ACETONITRILESOLUTION

### IATA

UN number: 1648 Class: 3 Packing group: II  
Proper shipping name: AcetonitrileSOLUTION



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**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 |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01    |

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard

**Massachusetts Right To Know Components**

|              | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01    |

**Pennsylvania Right To Know Components**

|              | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01    |

**New Jersey Right To Know Components**

|              | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01    |

**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.

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**SECTION 16: Other information****Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://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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