1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers
Product name : 1-Phenylethan-1-d1-ol
Product Number : 614963
Brand : Aldrich
CAS-No. : 3101-96-0

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified uses : Laboratory chemicals, Manufacture 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 # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318

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)
H227 Combustible liquid
H302 Harmful if swallowed.
H315 Causes skin irritation.
H318 Causes serious eye damage.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you
feel unwell.

P302 + P352
IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P310
Immediately call a POISON CENTER or doctor/physician.

P321
Specific treatment (see supplemental first aid instructions on this label).

P330
Rinse mouth.

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 for extinction.

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical characterization: Isotopically labeled

Synonyms: sec-Phenethyl-α-d1 alcohol
sec-Phenethyl-α-d1 alcohol

Formula: C₈DH₉O

Molecular Weight: 123.17 g/mol

CAS-No.: 3101-96-0

<table>
<thead>
<tr>
<th>Hazardous components</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Phenylethan-1-d₁-ol</td>
<td>Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; H227, H302, H315, H318</td>
<td>-</td>
</tr>
</tbody>
</table>

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
5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

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). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. 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
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

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contains no substances with occupational exposure limit values.

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, 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.

---

**9. PHYSICAL AND CHEMICAL PROPERTIES**

**9.1 Information on basic physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form: Appearance</td>
<td>clear, liquid</td>
</tr>
<tr>
<td>Colour</td>
<td>colourless</td>
</tr>
<tr>
<td>Odour</td>
<td>no data available</td>
</tr>
<tr>
<td>Odour Threshold</td>
<td>no data available</td>
</tr>
<tr>
<td>pH</td>
<td>no data available</td>
</tr>
<tr>
<td>Melting point/freezing point</td>
<td>19 - 20 °C (66 - 68 °F) - lit.</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>204 °C (399 °F) at 993 hPa (745 mmHg) - lit.</td>
</tr>
<tr>
<td>Flash point</td>
<td>86 °C (187 °F) - closed cup</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>no data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>no data available</td>
</tr>
<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>no data available</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>no data available</td>
</tr>
<tr>
<td>Vapour density</td>
<td>no data available</td>
</tr>
<tr>
<td>Relative density</td>
<td>1.02 g/mL at 25 °C (77 °F)</td>
</tr>
<tr>
<td>Water solubility</td>
<td>1.02 g/cm3 at 25 °C (77 °F)</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>no data available</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>no data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>no data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>no data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>no data available</td>
</tr>
</tbody>
</table>
t) Oxidizing properties no data available

9.2 Other safety information no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity no data available

10.2 Chemical stability Stable 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 Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity no data available
Inhalation: no data available
Dermal: no data available

Skin corrosion/irritation no data available

Serious eye damage/eye irritation

Respiratory or skin sensitisation no data available

Germ cell mutagenicity

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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
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
burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting
Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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.

14. TRANSPORT INFORMATION

DOT (US)
UN number: 2937 Class: 6.1 Packing group: III
Proper shipping name: alpha-Methylbenzyl alcohol, liquid
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG
UN number: 2937 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: alpha-METHYLBENZYL ALCOHOL, LIQUID
Marine pollutant: No

IATA
UN number: 2937 Class: 6.1 Packing group: III
Proper shipping name: alpha-Methylbenzyl alcohol, liquid

15. REGULATORY INFORMATION

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

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>3101-96-0</td>
<td>2007-03-01</td>
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</table>

**New Jersey Right To Know Components**

<table>
<thead>
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<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>3101-96-0</td>
<td>2007-03-01</td>
</tr>
</tbody>
</table>

**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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**16. OTHER INFORMATION**

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

- Acute Tox.: Acute toxicity
- Eye Dam.: Serious eye damage
- Flam. Liq.: Flammable liquids
- H227: Combustible liquid
- H302: Harmful if swallowed.
- H315: Causes skin irritation.
- H318: Causes serious eye damage.
- Skin Irrit.: Skin irritation

**HMIS Rating**
- Health hazard: 2
- Chronic Health Hazard: *
- Flammability: 2
- Physical Hazard: 0

**NFPA Rating**
- Health hazard: 2
- Fire Hazard: 2
- Reactivity Hazard: 0

**Further information**
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**Preparation Information**
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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