

SAFETY DATA SHEET

Version 5.1
Revision Date 07/10/2014
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1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 1-Pentan-d₁₁-ol

Product Number : 491276

Brand : Aldrich

CAS-No. : 126840-22-0

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 # : +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 liquids (Category 3), H226

Acute toxicity, Inhalation (Category 4), H332

Skin irritation (Category 2), H315

Serious eye damage (Category 1), H318

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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)

H226

Flammable liquid and vapour.

H315

Causes skin irritation.

H318

Causes serious eye damage.

H332

Harmful if inhaled.

H335

May cause respiratory 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.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
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).
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 + 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Chemical characterization : Isotopically labeled
Synonyms : Pentyl-d11 alcohol

Formula : C₅D₁₁HO
Molecular Weight : 99.22 g/mol
CAS-No. : 126840-22-0

Hazardous components

Component	Classification	Concentration
1-Pentan-d11-ol		
	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H315, H318, H332, H335	-

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

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 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).

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, 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.

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	Melting point/range: -78 °C (-108 °F) - lit.
f) Initial boiling point and boiling range	136 - 138 °C (277 - 280 °F) - lit.
g) Flash point	49.00 °C (120.20 °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: 10.00 %(V) Lower explosion limit: 1.20 %(V)
k) Vapour pressure	2.0 hPa (1.5 mmHg) at 20.00 °C (68.00 °F)
l) Vapour density	no data available
m) Relative density	0.911 g/mL at 25 °C (77 °F) 0.911 g/cm ³ at 25 °C (77 °F)
n) Water solubility	no data available
o) Partition coefficient: n-octanol/water	log Pow: 1.510
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

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

no data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents, Alkali metals, Strong acids, Halides, Aldehydes

10.6 Hazardous decomposition products

no data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - mouse - 200 mg/kg

Remarks: Behavioral:General anesthetic.

LD50 Oral - rat - 3,670 mg/kg

LD50 Dermal - rabbit - 2,306 mg/kg

Remarks: Liver:Other changes. Kidney, Ureter, Bladder:Other changes.

no data available

Skin corrosion/irritation

Skin - rabbit

Result: Skin irritation - 24.00 h

Serious eye damage/eye irritation

Eyes - rabbit

Result: Severe eye irritation - 24.00 h

Respiratory or skin sensitisation

Did not cause sensitisation on laboratory animals.

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.

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

no data available

no data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish LC50 - Oncorhynchus mykiss (rainbow trout) - 370 - 490 mg/l - 96.0 h

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

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.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1105 Class: 3 Packing group: III
Proper shipping name: Pentanols
Reportable Quantity (RQ):
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

UN number: 1105 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: PENTANOLS
Marine pollutant: No

IATA

UN number: 1105 Class: 3 Packing group: III

Proper shipping name: Pentanols

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

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1-Pentan-d11-ol	126840-22-0	

New Jersey Right To Know Components

	CAS-No.	Revision Date
1-Pentan-d11-ol	126840-22-0	

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.

Acute Tox.	Acute toxicity
Eye Dam.	Serious eye damage
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
Skin Irrit.	Skin irritation
STOT SE	Specific target organ toxicity - single exposure

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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