

SAFETY DATA SHEET

Version 6.6
Revision Date 10/08/2021
Print Date 06/01/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Benzyl-2,3,4,5,6-d₅ cyanide

Product Number : 495859
Brand : Aldrich
CAS-No. : 70026-36-7

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 ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +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)**

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 2), H330
Acute toxicity, Dermal (Category 3), H311

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)
H301 + H311 : Toxic if swallowed or in contact with skin.

H330	Fatal if inhaled.
Precautionary statement(s)	
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.
P280	Wear protective gloves/ protective clothing.
P284	Wear respiratory protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P310	Immediately call a POISON CENTER/ doctor.
P320	Specific treatment is urgent (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P361	Remove/ Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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

3.1 Substances

Formula	: C ₈ D ₅ H ₂ N
Molecular weight	: 122.13 g/mol
CAS-No.	: 70026-36-7

Component	Classification	Concentration
BENZYL-2,3,4,5,6-D5 CYANIDE		
	Acute Tox. 3; Acute Tox. 2; Acute Tox. 3; H301, H330, H311	<= 100 %

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. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

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**

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_x)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe 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

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

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.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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
BENZYL-2,3,4,5,6-D5 CYANIDE	70026-36-7	TWA	5 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	Remarks	Skin designation		
		C	5 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		TWA	5 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		C	4.7 ppm 5 mg/m ³	USA. NIOSH Recommended Exposure Limits

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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, 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.

SECTION 9: Physical and chemical properties**9.1 Information on basic physical and chemical properties**

- | | |
|---|--|
| a) Appearance | Form: liquid |
| b) Odor | unpleasant |
| c) Odor Threshold | No data available |
| d) pH | 11.0 - 12.0 at 117.2 g/l at 25 °C (77 °F) |
| e) Melting point/freezing point | Melting point/range: -24 °C (-11 °F) - lit. |
| f) Initial boiling point and boiling range | 233 - 234 °C 451 - 453 °F - lit. |
| g) Flash point | 102 °C (216 °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 | 0.1 hPa at 20 °C (68 °F)
1.1 hPa at 55 °C(131 °F)
1 hPa at 81.7 °C(179.1 °F) |
| l) Vapor density | 4.69 |
| m) Density | 1.059 g/cm ³ at 25 °C (77 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | 117.2 g/l at 20 °C (68 °F) |
| o) Partition coefficient: n-octanol/water | log Pow: 1.56 |

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p) Autoignition 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

Relative vapor density	4.69
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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

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents, Carbon dioxide (CO₂)

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD₅₀ Oral - Rat - 270 mg/kg

Remarks: Behavioral:Convulsions or effect on seizure threshold.

Lungs, Thorax, or Respiration:Dyspnea.

Liver:Other changes.

LC₅₀ Inhalation - Rat - 2 h - 430 mg/m³

Remarks: Behavioral:Altered sleep time (including change in righting reflex).

Behavioral:Muscle contraction or spasticity.

Lungs, Thorax, or Respiration:Dyspnea.

LD₅₀ Dermal - Rabbit - 270 mg/kg

LD₅₀ Dermal - 1,000 mg/kg

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation

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

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

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, Cyanosis, Mydriasis., Central nervous system depression, Coma., Seizures., Cushing's syndrome

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish LC0 - Leuciscus idus (Golden orfe) - 50 mg/l - 48 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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 2470 Class: 6.1 Packing group: III
Proper shipping name: Phenylacetonitrile, liquid
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2470 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: PHENYLACETONITRILE, LIQUID

IATA

UN number: 2470 Class: 6.1 Packing group: III
Proper shipping name: Phenylacetonitrile, liquid

SECTION 15: Regulatory information

SARA 302 Components

The following components are subject to reporting levels established by SARA Title III, Section 302:

BENZYL-2,3,4,5,6-D5 CYANIDE

CAS-No.
70026-36-7

Revision Date
2008-11-03

SARA 313 Components

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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

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

BENZYL-2,3,4,5,6-D5 CYANIDE	CAS-No. 70026-36-7	Revision Date 2008-11-03
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Pennsylvania Right To Know Components

BENZYL-2,3,4,5,6-D5 CYANIDE	CAS-No. 70026-36-7	Revision Date 2008-11-03
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New Jersey Right To Know Components

BENZYL-2,3,4,5,6-D5 CYANIDE	CAS-No. 70026-36-7	Revision Date 2008-11-03
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California Prop. 65 Components

WARNING: This product contains a chemical known in the State of California to cause birth defects or other reproductive harm. BENZYL-2,3,4,5,6-D5 CYANIDE	CAS-No. 70026-36-7	Revision Date
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SECTION 16: Other information

Further information

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