

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.6
Revision Date 07/16/2026
Print Date 07/17/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Benzyl cyanide-(cyano-¹³C)

Product Number : 486965
Brand : Aldrich
CAS-No. : 83552-81-2

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

Identified uses : Laboratory chemicals, Synthesis of substances
Restrictions on use : Not Available

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral) : Category 3
Acute toxicity (Inhalation) : Category 1

Acute toxicity (Dermal) : Category 3

Short-term (acute) : Category 3
aquatic hazard

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H301 + H311 Toxic if swallowed or in contact with skin.
H330 Fatal if inhaled.
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**

P260 Do not breathe mist or vapours.
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.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing.
P284 Wear respiratory protection.

Response:

P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P352 + P312 IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P362 Take off contaminated clothing and wash before reuse.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Aldrich - 486965

Page 2 of 15

Substance / Mixture : Substance
CAS-No. : 83552-81-2

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Benzyl cyanide-cyano-13C	83552-81-2*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves.
Show this safety data sheet to the doctor in attendance.
- If inhaled : After inhalation: fresh air. Immediately call in physician.
If breathing stops: immediately apply artificial respiration, if necessary also oxygen.
- In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
Call a physician immediately.
- In case of eye contact : After eye contact: rinse out with plenty of water.
Remove contact lenses.
- If swallowed : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.
- Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.
	Vapours are heavier than air and may spread along floors.
	Forms explosive mixtures with air on intense heating.
	Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides Nitrogen oxides (NO _x)
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency
---	---

procedures, consult an expert.
Advice for emergency responders:
Wear appropriate personal protective equipment, as indicated in Section 8.

- Environmental precautions : Do not let product enter drains.
- Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

- Advice on safe handling : Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
- Further information on storage conditions : Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
- Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Benzyl cyanide-cyano-13C	83552-81-2	TWA	5 mg/m ³ (Cyanide)	OSHA Z-1
		C	4.7 ppm 5 mg/m ³ (Cyanide)	NIOSH REL

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : butyl-rubber
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Butoject® (KCL 898)

Material : Nitrile rubber
Break through time : 10 min
Glove thickness : 0.4 mm
Protective index : Splash contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Colour : light yellow

Odour : No data available

Odour Threshold : No data available
pH : No data available

Melting point/ range : -11 °F / -24 °C
Method: lit.

Boiling point/boiling range : 451 - 453 °F / 233 - 234 °C
Method: lit.

Flash point : 215.60 °F / 102.00 °C
Method: closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /
Upper flammability limit : No data available

Lower explosion limit /
Lower flammability limit : No data available

Vapour pressure : 1 hPa (131.00 °F / 55.00 °C)

Relative vapour density : No data available

Relative density : No data available

Density : 1.024 g/mL (77 °F / 25 °C)
1.024 g/cm³ (77 °F / 25 °C)

Water solubility	: No data available
Partition coefficient: n-octanol/water	: log Pow: 1.560 Bioaccumulation is not expected.
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 118.14 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: strong alkalis Oxidizing agents Reducing agents acids
Conditions to avoid	: Strong heating.
Incompatible materials	: No data available
Hazardous decomposition products	: For Hazardous combustion products in the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 210 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: benzyl cyanide

Acute toxicity estimate Inhalation - 4 h - 0.051 mg/l - vapour

(Expert judgement)

Remarks: The GHS classification specified by the authority

The value is given in analogy to the following substances: benzyl cyanide

LD50 Dermal - Rabbit - 270 mg/kg

Remarks: (RTECS)

The value is given in analogy to the following substances: benzyl cyanide

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Chromosome aberration test in vitro

Test system: lymphocyte

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Remarks: Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: **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

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

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

Systemic effects:

After absorption:

Cough
Dizziness
Headache
Nausea
agitation, spasms
Unconsciousness
respiratory arrest

Effect of the decomposition products.

After absorption:

Shortness of breath
Vomiting
CNS disorders
depressed respiration
Coma

Chronic intoxication:

Changes in the blood count

Damage to:

Central nervous system
Lungs

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Benzyl cyanide-cyano-13C:

- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 57 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: benzyl cyanide
- Toxicity to algae/aquatic plants : NOEC (Selenastrum capricornutum (green algae)): 117 mg/l
Exposure time: 4 Days
Remarks: (ECHA)
The value is given in analogy to the following substances:
The value is given in analogy to the following substances: benzyl cyanide

Ecotoxicology Assessment

- Chronic aquatic toxicity : This product has no known ecotoxicological effects.
The value is given in analogy to the following substances: benzyl cyanide

Persistence and degradability

Components:

Benzyl cyanide-cyano-13C:

- Biodegradability : Inoculum: activated sludge
Result: Readily biodegradable.
Biodegradation: 77 %
Exposure time: 14 d
Method: OECD Test Guideline 301C
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: benzyl cyanide

Bioaccumulative potential

Components:

Benzyl cyanide-cyano-13C:

Partition coefficient: n-octanol/water : log Pow: 1.560
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

No data available

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 2470
Proper shipping name : Phenylacetonitrile, liquid
Class : 6.1
Packing group : III
Labels : Division 6.1 - Toxic substances
Packing instruction (cargo aircraft) : 663
Packing instruction (passenger aircraft) : 655

IMDG-Code

UN number : UN 2470
Proper shipping name : PHENYLACETONITRILE, LIQUID

Class : 6.1
Packing group : III
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

Aldrich - 486965

Page 12 of 15

National Regulations

49 CFR

UN/ID/NA number : UN 2470
Proper shipping name : Phenylacetone nitrile, liquid

Class : 6.1

Packing group : III
Labels : Division 6.1 - Toxic substances
ERG Code : 152
Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Benzyl cyanide-cyano-13C	83552-81-2	500	500

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
Benzyl cyanide-cyano-13C	83552-81-2	500

SARA 311/312 Hazards : Acute Health Hazard

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.

US State Regulations

Massachusetts Right To Know

Benzyl cyanide-cyano-13C 83552-81-2

Pennsylvania Right To Know

Benzyl cyanide-cyano-13C 83552-81-2

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

NIOSH REL : USA. NIOSH Recommended Exposure Limits
OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
NIOSH REL / C : Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA : 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and

Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2025 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Revision Date : 07/16/2026

US / EN