

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.8
Revision Date 07/13/2026
Print Date 07/14/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Benzoic acid-2,3,4,5,6-d₅

Product Number : 217158
Brand : Aldrich
CAS-No. : 1079-02-3

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Skin irritation : Category 2

Serious eye damage : Category 1

Specific target organ toxicity - repeated exposure (Inhalation) : Category 1 (Lungs)

Short-term (acute) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H315 Causes skin irritation.
H318 Causes serious eye damage.
H372 Causes damage to organs (Lungs) through prolonged or repeated exposure if inhaled.
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**
P260 Do not breathe dust.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.

Response:
P302 + P352 IF ON SKIN: Wash with plenty of water.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P314 Get medical advice/ attention if you feel unwell.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Aldrich - 217158

Page 2 of 16

Substance / Mixture : Substance

CAS-No. : 1079-02-3

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Benzoic acid-d5	1079-02-3*	>= 80 - <= 100	TSC

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact : After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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 : Water
Foam
Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products : Carbon oxides

Specific extinguishing methods : No data available

Further information : 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:
Avoid generation and inhalation of dusts in all circumstances.
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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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.
- Further information on storage conditions : Tightly closed.
Dry.
Keep in a well-ventilated place.
Keep locked up or in an area accessible only to qualified or authorised persons.
- Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
- Recommended storage temperature : Recommended storage temperature see product label.
- Further information on storage stability : Store under inert gas.
hygroscopic

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Benzoic acid-d5	1079-02-3	TWA (Inhalable fraction and vapor)	0.5 mg/m ³	ACGIH

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts 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 P2

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 : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

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).
Tightly fitting safety goggles

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 : solid

Colour : No data available

Odour : No data available

Odour Threshold : No data available
pH : No data available

Melting point/ range	: 250 - 257 °F / 121 - 125 °C Method: lit.
Boiling point/boiling range	: 480 °F / 249 °C Method: lit.
Flash point	: Not applicable
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	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n- octanol/water	: No data available
Autoignition temperature	: 1062 °F / 572 °C
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 127.11 g/mol

Particle characteristics
Particle size : No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : Risk of ignition or formation of inflammable gases or vapours with:
Fluorine
Exothermic reaction with:
bases
Strong oxidizing agents
Strong bases
nitrites
strong reducing agents

Conditions to avoid : Avoid moisture.

no information available

Incompatible materials : No data available

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 - Mouse - male and female - 2,250 mg/kg
(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: Benzoic acid

Symptoms: Nausea, Vomiting, Irritation of mucous membranes

LC50 Inhalation - Rat - male and female - 4 h - > 12.2 mg/l - dust/mist

Remarks: (ECHA)

The value is given in analogy to the following substances: Benzoic acid

Symptoms: Cough, Possible damages:, mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg

Remarks: (ECHA)

The value is given in analogy to the following substances: Benzoic acid

Skin corrosion/irritation

Skin - Guinea pig

Result: Skin irritation - 3 h

Remarks: (ECHA)

The value is given in analogy to the following substances: Benzoic acid

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive - 21 Days

(Directive 67/548/EEC, Annex V, B.5.)

Remarks: The value is given in analogy to the following substances: Benzoic acid

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

Remarks: (ECHA)

The value is given in analogy to the following substances: Benzoic acid

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster fibroblasts

Metabolic activation: without metabolic activation

Result: Positive results were obtained in some in vitro tests.

Remarks: (ECHA)

The value is given in analogy to the following substances: Benzoic acid

Test Type: Micronucleus test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 487

Result: negative

Remarks: The value is given in analogy to the following substances: Benzoic acid

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

Inhalation - Causes damage to organs through prolonged or repeated exposure.

- Lungs

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

The value is given in analogy to the following substances: Benzoic acid

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - inhalation (dust/mist/fume) - 28 Days

Remarks: The value is given in analogy to the following substances: Benzoic acid

Repeated dose toxicity - Rabbit - male and female - Dermal - 21 Days - No observed adverse effect level - > 2,500 mg/kg

Remarks: The value is given in analogy to the following substances: Benzoic acid

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

SECTION 12. ECOLOGICAL INFORMATION**Ecotoxicity****Components:****Benzoic acid-d5:**

Toxicity to fish	: LC50 (<i>Lepomis macrochirus</i>): 44.6 mg/l End point: mortality Exposure time: 96 h Test Type: static test Method: US-EPA Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: Benzoic acid
Toxicity to daphnia and other aquatic invertebrates	: LC50 (<i>Daphnia magna</i> (Water flea)): > 100 mg/l End point: mortality Exposure time: 48 h Test Type: static test Method: US-EPA Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following substances: Benzoic acid
Toxicity to algae/aquatic plants	: ErC50 (<i>Pseudokirchneriella subcapitata</i>): > 33.1 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes Remarks: The value is given in analogy to the following substances: The value is given in analogy to the following

Aldrich - 217158

Page 10 of 16

substances: Benzoic acid

Toxicity to fish (Chronic toxicity) : EC50 (Oncorhynchus mykiss (rainbow trout)): > 120 mg/l

Exposure time: 28 d

Test Type: semi-static test

Method: OECD Test Guideline 204

Remarks: The value is given in analogy to the following substances:

The value is given in analogy to the following substances: Benzoic acid

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : EC50 (Daphnia magna (Water flea)): > 25 mg/l

Exposure time: 21 d

Test Type: semi-static test

Method: OECD Test Guideline 211

Remarks: The value is given in analogy to the following substances:

The value is given in analogy to the following substances: Benzoic acid

Toxicity to microorganisms : IC50 (activated sludge): > 1,000 mg/l

Exposure time: 3 h

Test Type: static test

Method: OECD Test Guideline 209

Remarks: The value is given in analogy to the following substances:

The value is given in analogy to the following substances: Benzoic acid

EC50 (Photobacterium phosphoreum): 17 mg/l

Exposure time: 30 min

Test Type: microtox test

Remarks: (Lit.)

The value is given in analogy to the following substances:

The value is given in analogy to the following substances: Benzoic acid

Ecotoxicology Assessment

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

Benzoic acid-d5:

Biodegradability : anaerobic
Inoculum: activated sludge
Result: Biodegradable
Biodegradation: 89.5 %

Exposure time: 35 d
Method: OECD Test Guideline 311
Remarks: The value is given in analogy to the following substances:
The value is given in analogy to the following substances: Benzoic acid

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects**Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:**Benzoic acid-d5:**

Results of PBT and vPvB assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

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**

Not regulated as a dangerous good

IMDG-Code

Aldrich - 217158

Page 12 of 16

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 3077
Proper shipping name : Environmentally hazardous substance, solid, n.o.s.
(Benzoic acid-d5)
Class : 9

Packing group : III
Labels : Class 9 - Miscellaneous dangerous substances and
articles
ERG Code : 171
Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of
transport regulations.

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

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Benzoic acid-d5	1079-02-3	5000	5000

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61). This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F). The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

Benzoic acid-d5	1079-02-3	>= 90 - <= 100 %
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Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

Benzoic acid-d5	1079-02-3	>= 90 - <= 100 %
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The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

Benzoic acid-d5	1079-02-3	>= 90 - <= 100 %
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This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

Benzoic acid-d5	1079-02-3
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Pennsylvania Right To Know

Benzoic acid-d5	1079-02-3
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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

Aldrich - 217158

Page 14 of 16

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE
SIGMA**

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
ACGIH / 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.

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Details in analogy to the undeuterated compound.

Revision Date : 07/13/2026

US / EN

Aldrich - 217158

Page 16 of 16

The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

MILLIPORE
SIGMA