

SAFETY DATA SHEET

Version 6.7
Revision Date 09/06/2024
Print Date 09/07/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 2,4-Dimethylphenol-3,5,6-d₃

Product Number : 613975
Brand : Aldrich
CAS-No. : 93951-75-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : 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

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, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318

Skin sensitization (Sub-category 1B), H317
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

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 Statements

H301 + H311

Toxic if swallowed or in contact with skin.

H314

Causes severe skin burns and eye damage.

H317

May cause an allergic skin reaction.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P260

Do not breathe dust.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P272

Contaminated work clothing must not be allowed out of the workplace.

P273

Avoid release to the environment.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

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.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P391

Collect spillage.

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 : C₈D₃H₇O
Molecular weight : 125.13 g/mol
CAS-No. : 93951-75-8

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EC-No. : 693-749-3

| Component | Classification | Concentration |
|------------------------------------|--|---------------|
| 2,4-Dimethylphenol-3,5,6-d3 | | |
| | Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1B; Aquatic Acute 2; Aquatic Chronic 2; H301, H311, H314, H318, H317, H401, H411 | <= 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

First aiders need to protect themselves. Show this material 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. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. 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. Do not attempt to neutralise.

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

Water Foam Carbon dioxide (CO₂) Dry powder

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Unsuitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

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

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 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.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1A: 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 |
|-----------------------------|------------|--|--------------------|---|
| 2,4-Dimethylphenol-3,5,6-d3 | 93951-75-8 | TWA | 1 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Dermal Sensitization Confirmed animal carcinogen with unknown relevance to humans | | |

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face 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 protection

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).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 30 min

Material tested: KCL 720 Camapren®

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A-(P3)

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.

required when dusts/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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: solid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: 22 - 23 °C (72 - 73 °F) Melting point/ range: 22 - 23 °C (72 - 73 °F) - lit. |
| f) Initial boiling point and boiling range | 211 - 212 °C 412 - 414 °F 211 - 212 °C (412 - 414 °F) - lit. |
| g) Flash point | ()Not applicable |
| 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 | No data available |
| l) Vapor density | No data available |
| m) Density | No data available |
| Relative density | No data available |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | No data available |
| 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 none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .
Stable

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents
Aluminum
Copper
various alloys

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

No data available

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

Acute toxicity estimate Oral - 100 mg/kg

(Expert judgment)

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: 2,4-xylenol; 2,4-dimethylphenol

Symptoms: mucosal irritations, Cough, Shortness of breath

Inhalation: Corrosive to respiratory system.

Acute toxicity estimate Dermal - 300 mg/kg

(Expert judgment)

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

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The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Skin corrosion/irritation

Remarks: Causes skin burns.

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

The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

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

The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and 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: 2,4-xylenol; 2,4-dimethylphenol

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

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

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

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After absorption:

CNS disorders

Damage to:

Liver

Kidney

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 4.21 mg/l - 48 h (OECD Test Guideline 202)
Remarks: The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata - 13 mg/l - 72 h (OECD Test Guideline 201)
Remarks: The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

Toxicity to fish(Chronic toxicity) NOEC - Pimephales promelas (fathead minnow) - 1.92 mg/l - 32 d
Remarks: (ECOTOX Database)
The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 98 % - Readily biodegradable.
(OECD Test Guideline 301C)
Remarks: The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

12.3 Bioaccumulative potential

Bioaccumulation Lepomis macrochirus (Bluegill) - 28 d
- 0.0102 mg/l(2,4-Dimethylphenol-3,5,6-d3)

Bioconcentration factor (BCF): 150
Remarks: The value is given in analogy to the following substances: 2,4-xylenol; 2,4-dimethylphenol

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

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

DOT (US)

UN number: 2261 Class: 6.1 Packing group: II
Proper shipping name: Xylenols, solid
Reportable Quantity (RQ): 100 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 2261 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: XYLENOLS, SOLID

IATA

UN number: 2261 Class: 6.1 Packing group: II
Proper shipping name: Xylenols, solid

SECTION 15: Regulatory information

CERCLA Reportable Quantity

| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|-----------------------------|------------|--------------------|-----------------------------|
| 2,4-Dimethylphenol-3,5,6-d3 | 93951-75-8 | 100 | 100 |

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 : The following components are subject to reporting levels established by SARA Title III, Section 313:

| | | |
|-----------------------------|------------|------------------|
| 2,4-Dimethylphenol-3,5,6-d3 | 93951-75-8 | >= 90 - <= 100 % |
|-----------------------------|------------|------------------|

US State Regulations

Massachusetts Right To Know

| | |
|-----------------------------|------------|
| 2,4-Dimethylphenol-3,5,6-d3 | 93951-75-8 |
|-----------------------------|------------|

Pennsylvania Right To Know

| | |
|-----------------------------|------------|
| 2,4-Dimethylphenol-3,5,6-d3 | 93951-75-8 |
|-----------------------------|------------|

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 ingredients of this product are reported in the following inventories:

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

Further information

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.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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