

SAFETY DATA SHEET

Version 6.3
Revision Date 09/17/2021
Print Date 06/01/2022

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

Product name : Phenol-2,4,6-d₃OD

Product Number : 591742
Brand : Aldrich
Index-No. : 604-001-00-2
CAS-No. : 80441-87-8

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 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Germ cell mutagenicity (Category 2), H341
Specific target organ toxicity - repeated exposure (Category 2), H373
Short-term (acute) aquatic hazard (Category 3), H402
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

Aldrich - 591742

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Pictogram



Signal word

Danger

Hazard statement(s)

H301 + H311 + H331

H314

H341

H373

Toxic if swallowed, in contact with skin or if inhaled.

Causes severe skin burns and eye damage.

Suspected of causing genetic defects.

May cause damage to organs through prolonged or repeated exposure.

H402

Harmful to aquatic life.

H411

Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

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.

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.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P391

Collect spillage.

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 : $C_6D_4H_2O$
Molecular weight : 98.06 g/mol
CAS-No. : 80441-87-8
Index-No. : 604-001-00-2

Component	Classification	Concentration
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Phenol-2,4,6-d3,OD		
	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Muta. 2; STOT RE 2; Aquatic Acute 3; Aquatic Chronic 2; H301, H331, H311, H314, H318, H341, H373, H402, 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

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

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

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

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

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 dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. 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. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 formation of dust and aerosols.

Advice on protection against fire and explosion

Provide appropriate exhaust ventilation at places where dust is formed.

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.

Store under inert gas. hygroscopic

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
Phenol-2,4,6-d3,OD	80441-87-8	TWA	5 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	5 ppm 19 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		C	15.6 ppm 60 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	5 ppm 19 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		TWA	5 ppm 19 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		PEL	5 ppm 19 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Phenol-2,4,6-d3,OD	80441-87-8	Phenol	250mg/g Creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

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.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.2 mm
Break through time: 30 min
Material tested: Dermatrill® P (KCL 743 / Aldrich Z677388, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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 particle respirator type N100 (US) or type P3 (EN 143) 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. Discharge into the environment must be avoided.

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 | 6 |
| e) Melting point/freezing point | Melting point/range: 40 - 42 °C (104 - 108 °F) - lit. |
| f) Initial boiling point and boiling range | 182 °C 360 °F - lit. |
| g) Flash point | 79 °C (174 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower | Upper explosion limit: 8.6 %(V) |

	flammability or explosive limits	Lower explosion limit: 1.7 %(V)
k)	Vapor pressure	6.20 hPa at 55 °C (131 °F) 0.48 hPa at 20 °C(68 °F)
l)	Vapor density	No data available
m)	Density	1.116 g/cm ³ at 25 °C (77 °F)
	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	log Pow: 1.46
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

Surface tension	38.2 mN/m at 50 °C (122 °F)
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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

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

LD50 Oral - 100.0 mg/kg

Oral: No data available

Inhalation: No data available

LC50 Inhalation - 4.0 h - 0.51 mg/l

Dermal: No data available

LD50 Dermal - 300.0 mg/kg

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

In vitro tests showed mutagenic effects

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

May cause damage to organs through prolonged or repeated exposure. **Aspiration hazard**
No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated., 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, Circulatory collapse, tachypnea, paralysis, Convulsions, Coma., necrosis of mouth and G.I. Tract, Jaundice, respiratory failure, cardiac arrest

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish LC50 - Carassius auratus (goldfish) - 36.1 - 68.8 mg/l - 96 h

Toxicity to daphnia EC50 - Daphnia magna (Water flea) - 12 mg/l - 24 h

and other aquatic
invertebrates

EC100 - Daphnia magna (Water flea) - 100 mg/l - 24 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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Harmful to aquatic life.

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: 1671 Class: 6.1 Packing group: II
Proper shipping name: Phenol, solid
Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1671 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: PHENOL, SOLID
Marine pollutant : yes

IATA

UN number: 1671 Class: 6.1 Packing group: II
Proper shipping name: Phenol, solid

SECTION 15: Regulatory information

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SARA 302 Components

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

Phenol-2,4,6-d3,OD

CAS-No.
80441-87-8

Revision Date
2007-07-01

SARA 313 Components

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

Phenol-2,4,6-d3,OD

CAS-No.
80441-87-8

Revision Date
2007-07-01

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

Phenol-2,4,6-d3,OD

CAS-No.
80441-87-8

Revision Date
2007-07-01

Pennsylvania Right To Know Components

Phenol-2,4,6-d3,OD

CAS-No.
80441-87-8

Revision Date
2007-07-01

California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

SECTION 16: Other information

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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