

SAFETY DATA SHEET

Version 6.7
Revision Date 03/04/2024
Print Date 03/23/2024

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

Product name : Phenol-2,3,4,5,6-d₅
Product Number : 425370
Brand : Aldrich
Index-No. : 604-001-00-2
CAS-No. : 4165-62-2

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, Inhalation (Category 3), H331
Skin corrosion (Category 1B), H314

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Serious eye damage (Category 1), H318
 Germ cell mutagenicity (Category 2), H341
 Specific target organ toxicity - repeated exposure (Category 2), Nervous system, Kidney, Liver, Skin, H373
 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 + H331

Toxic if swallowed or if inhaled.

H314

Causes severe skin burns and eye damage.

H341

Suspected of causing genetic defects.

H373

May cause damage to organs (Nervous system, Kidney, Liver, Skin) through prolonged or repeated exposure.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P201

Obtain special instructions before use.

P202

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

P260

Do not breathe dust.

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.

P363

Wash contaminated clothing 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

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SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C₆D₅HO
Molecular weight : 99.04 g/mol
CAS-No. : 4165-62-2
EC-No. : 685-274-5
Index-No. : 604-001-00-2

Component	Classification	Concentration
Phenol-2,3,4,5,6-d5		
	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Muta. 2; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301, H331, H314, H318, H341, H373, 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. 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. 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

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.

Vapors 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.

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

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

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
Phenol-2,3,4,5,6-d5	4165-62-2	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/m ³	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		C	15.6 ppm 60 mg/m ³	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	5 ppm 19 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		

		PEL	5 ppm 19 mg/m ³	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-2,3,4,5,6-d5	4165-62-2	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

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: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Body Protection

Flame retardant antistatic 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: 40 - 42 °C (104 - 108 °F) Melting point/range: 40 - 42 °C (104 - 108 °F) - lit.
f) Initial boiling point and boiling range	182 °C 360 °F 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 flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.127 g/mL at 25 °C (77 °F)1.127 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	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

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

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) .

10.3 Possibility of hazardous reactions

Exothermic reaction with:

Aluminum

Aldehydes

halogens

hydrogen peroxide

iron(III) compounds

Oxidizing agents

Strong acids

Strong bases

formaldehyde

Risk of explosion with:

nitrites

nitrates

salts of oxyhalogenic acids

peroxi compounds

10.4 Conditions to avoid

Strong heating.

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 - 100.1 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: Phenol

Acute toxicity estimate Inhalation - 0.51 mg/l - dust/mist

(Expert judgment)

Symptoms: Irritation, Lung edema

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: Phenol

Dermal: No data available

Skin corrosion/irritation

Skin - In vitro study

Result: Causes burns.

(OECD Test Guideline 431)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive

(OECD Test Guideline 405)

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

Remarks: Causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

Remarks: (IUCLID)

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

Germ cell mutagenicity

Suspected of causing genetic defects.

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

Test system: Chinese hamster ovary cells

Metabolic activation: Metabolic activation

Method: OECD Test Guideline 473

Result: positive

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

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 487

Result: positive

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

Phenol

Carcinogenicity
This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

- 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

May cause damage to organs through prolonged or repeated exposure.

- Nervous system, Kidney, Liver, Skin

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: Phenol

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, Circulatory collapse, tachypnea, paralysis, Convulsions, Coma., necrosis of mouth and G.I. Tract, Jaundice, respiratory failure, cardiac arrest

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - <i>Onchorhynchus clarki</i> - 8.9 mg/l - 96 h (US-EPA) Remarks: The value is given in analogy to the following substances: Phenol
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Ceriodaphnia dubia</i> (water flea) - 3.1 mg/l - 48 h (US-EPA) Remarks: The value is given in analogy to the following substances: Phenol

Toxicity to algae	static test EC50 - <i>Pseudokirchneriella subcapitata</i> (algae) - 61.1 mg/l - 96 h (US-EPA) Remarks: The value is given in analogy to the following substances: Phenol
Toxicity to bacteria	static test IC50 - microorganisms - 21 mg/l - 24 h Remarks: (ECHA) The value is given in analogy to the following substances: Phenol
Toxicity to fish(Chronic toxicity)	semi-static test NOEC - Fish - 0.077 mg/l - 60 d Remarks: (ECHA) The value is given in analogy to the following substances: Phenol
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - <i>Daphnia magna</i> (Water flea) - 0.16 mg/l - 16 d Remarks: (ECHA) The value is given in analogy to the following substances: Phenol

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 100 h Result: 62 % - Readily biodegradable. (OECD Test Guideline 301C) Remarks: The value is given in analogy to the following substances: Phenol
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12.3 Bioaccumulative potential

Bioaccumulation	Danio rerio (zebra fish) - 5 h at 25 °C - 2 mg/l(Phenol-2,3,4,5,6-d5) Bioconcentration factor (BCF): 17.5 (OECD Test Guideline 305) Remarks: Does not bioaccumulate. The value is given in analogy to the following substances: Phenol
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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

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: 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

SARA 302 Components

Phenol-2,3,4,5,6-d5	CAS-No. 4165-62-2	Revision Date 2007-07-01
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SARA 313 Components

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

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SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

Phenol-2,3,4,5,6-d5	CAS-No. 4165-62-2	Revision Date 2007-07-01
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Pennsylvania Right To Know Components

Phenol-2,3,4,5,6-d5

CAS-No.
4165-62-2

Revision Date
2007-07-01

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.

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