

## SAFETY DATA SHEET

Version 6.5  
Revision Date 09/13/2021  
Print Date 06/01/2022

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

Product name : Phenol- $^{13}\text{C}_6$

Product Number : 490504  
Brand : Aldrich  
Index-No. : 604-001-00-2  
CAS-No. : 89059-34-7

**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), 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 statement(s)

H301 + H311 + H331

Toxic if swallowed, in contact with skin 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 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 :  $^{13}\text{C}_6\text{H}_6\text{O}$   
Molecular weight : 100.01 g/mol  
CAS-No. : 89059-34-7  
Index-No. : 604-001-00-2

Component	Classification	Concentration
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Phenol-13C6		
	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Muta. 2; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301, H331, H311, H314, H318, H341, H373, H401, H411 Concentration limits: >= 3 %: Skin Corr. 1B, H314; 1 - < 3 %: Skin Irrit. 2, H315; 1 - < 3 %: Eye Irrit. 2, H319;	<= 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

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## **SECTION 5: Firefighting measures**

### **5.1 Extinguishing media**

#### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

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## **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.

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## **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-13C6	89059-34-7	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 <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		C	15.6 ppm 60 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	5 ppm 19 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		PEL	5 ppm 19 mg/m <sup>3</sup>	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-13C6	89059-34-7	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

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

Flame retardant antistatic protective clothing.

#### 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.

### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |               |              |
|---------------|--------------|
| a) Appearance | Form: powder |
|               | Color: white |

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	1.139 g/mL at 25 °C (77 °F) 1.139 g/cm <sup>3</sup> 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

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## 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

No data available

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#### 10.4 Conditions to avoid

Strong heating.

#### 10.5 Incompatible materials

rubber, various plastics, various alloys, various metals, Strong oxidizing agents

#### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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### SECTION 11: Toxicological information

#### 11.1 Information on toxicological effects

##### Acute toxicity

Oral: No data available

Inhalation: No data available

LD50 Dermal - Rat - female - 660 mg/kg

(OECD Test Guideline 402)

##### Skin corrosion/irritation

Skin - In vitro study

Result: Causes burns.

(OECD Test Guideline 431)

##### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive

(OECD Test Guideline 405)

Causes serious eye damage. Risk of blindness!

##### Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

Remarks: (IUCLID)

##### 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

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

##### 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

**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

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**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)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Ceriodaphnia dubia</i> (water flea) - 3.1 mg/l - 48 h (US-EPA)
Toxicity to algae	static test EC50 - <i>Pseudokirchneriella subcapitata</i> (algae) - 61.1 mg/l - 96 h (US-EPA)
Toxicity to bacteria	static test IC50 - microorganisms - 21 mg/l - 24 h Remarks: (ECHA)

**12.2 Persistence and degradability**

Biodegradability	aerobic - Exposure time 100 h Result: 62 % - Readily biodegradable. (OECD Test Guideline 301C)
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**12.3 Bioaccumulative potential**

Bioaccumulation	Danio rerio (zebra fish) - 5 h at 25 °C - 2 mg/l(Phenol-13C6)
	Bioconcentration factor (BCF): 17.5

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Remarks: Does not bioaccumulate.

#### 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

No data available

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### 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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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### 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

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### SECTION 15: Regulatory information

#### SARA 302 Components

Phenol-13C6

CAS-No.  
89059-34-7

Revision Date  
2007-07-01

#### SARA 313 Components

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

CAS-No.

Revision Date

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**SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

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**SECTION 16: Other information****Further information**

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](http://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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