

SAFETY DATA SHEET

Version 6.0
Revision Date 05/26/2018
Print Date 11/18/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 2-Chlorophenol-3,4,5,6-d<SB>4</>

Product Number : 449423
Brand : Aldrich

CAS-No. : 93951-73-6

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 Street
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Serious eye damage (Category 1), H318

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (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)	
H227	Combustible liquid.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H318	Causes serious eye damage.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ 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 + P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER/doctor.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Molecular weight : 132.50 g/mol
CAS-No. : 93951-73-6

Hazardous components

Component	Classification	Concentration
2-Chlorophenol-3,4,5,6-d4		
	Flam. Liq. 4; Acute Tox. 4; Eye Dam. 1; Aquatic Acute 2; Aquatic Chronic 2; H227, H302 + H312 + H332, H318, H411	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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

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, Hydrogen chloride gas

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Stench.

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: liquid, clear
Colour: light yellow |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 8 °C (46 °F) - lit. |
| f) Initial boiling point and boiling range | 175 - 176 °C (347 - 349 °F) - lit. |
| g) Flash point | 64 °C (147 °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) Vapour pressure | 1.3 hPa at 121.0 °C (249.8 °F) |
| l) Vapour density | No data available |
| m) Relative density | 1.279 g/cm ³ at 25 °C (77 °F) |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | log Pow: 5.0 |

octanol/water

- | | |
|------------------------------|-------------------|
| p) Auto-ignition 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

No data available

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

Heat, flames and sparks.

10.5 Incompatible materials

Acid chlorides, Acid anhydrides, Oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 670.0 mg/kg

LD50 Oral - Mouse - 345.0 mg/kg

Remarks: Behavioral:Tremor. Behavioral:Convulsions or effect on seizure threshold. Lungs, Thorax, or Respiration:Respiratory stimulation.

LD50 Oral - Mammal - 440.0 mg/kg

Remarks: Behavioral:Muscle weakness. Behavioral:Muscle contraction or spasticity. Sweating

Inhalation: No data available

Dermal: No data available

LD50 Intraperitoneal - Rat - 230 mg/kg

Remarks: Behavioral:Tremor. Behavioral:Convulsions or effect on seizure threshold. Nutritional and Gross Metabolic:Changes in:Body temperature increase.

LD50 Subcutaneous - Rat - 950 mg/kg

LD50 Intraperitoneal - Mouse - 235 mg/kg

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

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.
- 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.
- ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- 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.
- 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.
- 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

No data available

Aspiration hazard

No data available

Additional Information

RTECS: Not available

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, prolonged or repeated exposure can cause:, Tremors, Convulsions, 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

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

Toxicity to fish	LC50 - Lepomis macrochirus (Bluegill) - 5.7 - 12 mg/l - 96.0 h(2-Chlorophenol-3,4,5,6-d4)
	LC50 - Pimephales promelas (fathead minnow) - 6 - 16 mg/l - 96.0 h(2-Chlorophenol-3,4,5,6-d4)
	LC50 - Carassius auratus (goldfish) - 10.7 - 15.2 mg/l - 96.0 h(2-Chlorophenol-3,4,5,6-d4)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 6.30 - 17.90 mg/l - 24 h(2-Chlorophenol-3,4,5,6-d4)
	Immobilization EC50 - Daphnia magna (Water flea) - 3.91 mg/l - 48 h(2-

Chlorophenol-3,4,5,6-d4)
Toxicity to algae EC50 - Pseudokirchneriella subcapitata (green algae) - 70.00 mg/l - 96 h(2-Chlorophenol-3,4,5,6-d4)
EC50 - Chlorella vulgaris (Fresh water algae) - 170.00 mg/l - 96 h(2-Chlorophenol-3,4,5,6-d4)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

Bioaccumulation Lepomis macrochirus (Bluegill) - 28 d
- 0.00918 mg/l(2-Chlorophenol-3,4,5,6-d4)

Bioconcentration factor (BCF): 214

12.4 Mobility in soil

No data available(2-Chlorophenol-3,4,5,6-d4)

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

Toxic to aquatic life.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Contact a licensed professional waste disposal service to dispose of this material. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 2021 Class: 6.1 Packing group: III
Proper shipping name: Chlorophenols, liquid
Reportable Quantity (RQ) : 100 lbs

Poison Inhalation Hazard: No

IMDG

UN number: 2021 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: CHLOROPHENOLS, LIQUID

IATA

UN number: 2021 Class: 6.1 Packing group: III
Proper shipping name: Chlorophenols, liquid

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

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

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

	CAS-No.	Revision Date
2-Chlorophenol-3,4,5,6-d4	93951-73-6	1993-04-24

California Prop. 65 Components

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

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

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

H227	Combustible liquid.
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H312	Harmful in contact with skin.
H318	Causes serious eye damage.
H332	Harmful if inhaled.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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