

SAFETY DATA SHEET

Version 6.12
Revision Date 09/08/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Chloroform-d

Product Number : 151823
Brand : Aldrich
CAS-No. : 865-49-6

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 4), H302
Acute toxicity, Inhalation (Category 3), H331
Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319

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Carcinogenicity (Category 2), H351
 Reproductive toxicity (Category 2), H361
 Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336
 Specific target organ toxicity - repeated exposure, Oral (Category 1), Liver, Kidney, H372
 Short-term (acute) aquatic hazard (Category 3), H402

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

| | |
|------|--|
| H302 | Harmful if swallowed. |
| H315 | Causes skin irritation. |
| H319 | Causes serious eye irritation. |
| H331 | Toxic if inhaled. |
| H336 | May cause drowsiness or dizziness. |
| H351 | Suspected of causing cancer. |
| H361 | Suspected of damaging fertility or the unborn child. |
| H372 | Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure if swallowed. |
| H402 | Harmful to aquatic life. |

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 mist or vapors. |
| 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 + P330 | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. |
| P302 + P352 | IF ON SKIN: Wash with plenty of soap and water. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| P332 + P313 | If skin irritation occurs: Get medical advice/ attention. |
| P337 + P313 | If eye irritation persists: Get medical advice/ attention. |
| P362 | Take off contaminated clothing and wash before reuse. |
| 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

| | | |
|------------------|---|--------------------|
| Synonyms | : | Deuteriochloroform |
| Formula | : | CCl ₃ D |
| Molecular weight | : | 120.38 g/mol |
| CAS-No. | : | 865-49-6 |
| EC-No. | : | 212-742-4 |

| Component | Classification | Concentration |
|----------------------------------|---|---------------|
| Chloroform-D1-Deuteration | | |
| | Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; Repr. 2; STOT SE 3; STOT RE 1; Aquatic Acute 3; H302, H331, H315, H319, H351, H361, H336, H372, H402 | <= 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. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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 extinguishing measures that are appropriate to local circumstances and the surrounding environment.

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

Hydrogen chloride gas

Not combustible.

Ambient fire may liberate hazardous vapours.

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

Suppress (knock down) gases/vapors/mists with a water spray jet. 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: Do not breathe vapors, aerosols. 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

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Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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

Store under inert gas. Light sensitive. hygroscopic

Storage class

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

| Component | CAS-No. | Value | Control parameters | Basis |
|---------------------------|----------|--|---------------------------------|---|
| Chloroform-D1-Deuteration | 865-49-6 | TWA | 10 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Confirmed animal carcinogen with unknown relevance to humans | | |
| | | ST | 2 ppm 9.78 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential Occupational Carcinogen | | |
| | | C | 50 ppm 240 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | PEL | 2 ppm 9.78 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

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). Safety glasses

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: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 10 min

Material tested: Butoject® (KCL 898)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type AX

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 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: liquid, clear Color: colorless |
| b) Odor | characteristic |

| | |
|---|---|
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/ range: -64 °C (-83 °F) - lit. |
| f) Initial boiling point and boiling range | 60.9 °C 141.6 °F - lit. |
| g) Flash point | () - Regulation (EC) No. 440/2008, Annex, A.9 does not flash |
| 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 | ca.265.31 hPa at ca.25 °C (ca.77 °F) |
| l) Vapor density | No data available |
| m) Density | 1.500 g/cm ³ at 25 °C (77 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | 4.6 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6 |
| o) Partition coefficient: n-octanol/water | log Pow: 1.5 at 20 °C (68 °F) - Bioaccumulation is not expected. |
| p) Autoignition temperature | No data available |
| q) Decomposition temperature | Distillable in an undecomposed state at normal pressure. |
| r) Viscosity | No data available |
| s) Explosive properties | Not classified as explosive. |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Risk of explosion with:

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Ammonia
Amines
nitrogen oxides
bases
Oxygen
alkali amides
organic nitro compounds
Alcohols
alkali hydroxides
strong alkalis
Fluorine
peroxi compounds
Alkaline earth metals
Alkali metals
Powdered metals
Methanol
with
alcoholates
Methanol
with
strong alkalis
Iron
in powder form
various alloys
sensitive to shock
Methanol
with
Sodium hydroxide
magnesium
in powder form
Oxygen
with
alkali compounds
Aluminum
in powder form
Acetone
with
alkali compounds
Potassium
sensitive to shock
sodium
sensitive to shock
Violent reactions possible with:
phosphines
bis(dimethylamino)dimethyl tin
nonmetallic hydrogen compounds
Powdered metals
Light metals
Ketones
mineral acids
Strong oxidizing agents
semimetallic hydrogen compounds

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The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

MILLIPORE
SIGMA

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

LD50 Oral - Rat - male - 908 mg/kg

(OECD Test Guideline 401)

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

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor

(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: Chloroform

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (ECHA)

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

Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

Remarks: (ECHA)

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

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

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

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

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

Test Type: unscheduled DNA synthesis assay

Test system: Liver
Metabolic activation: without metabolic activation
Result: negative
Remarks: (ECHA)
The value is given in analogy to the following substances: Chloroform
Test Type: Micronucleus test
Species: Rat
Cell type: Red blood cells (erythrocytes)
Application Route: Oral
Method: OECD Test Guideline 474
Result: negative
Remarks: The value is given in analogy to the following substances: Chloroform

Test Type: unscheduled DNA synthesis assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Method: OECD Test Guideline 486
Result: negative
Remarks: The value is given in analogy to the following substances: Chloroform

Test Type: in vivo assay
Species: Mouse

Application Route: Inhalation

Result: negative
Remarks: (ECHA)
The value is given in analogy to the following substances: Chloroform

Carcinogenicity

Suspected of causing cancer.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Chloroform-D1-Deuteration)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Chloroform-D1-Deuteration)

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

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

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

Specific target organ toxicity - repeated exposure

Oral - Causes damage to organs through prolonged or repeated exposure.

- Liver, Kidney

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: Chloroform

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - female - Oral - NOAEL (No observed adverse effect level) - 34 mg/kg

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

Vomiting, Cough, irritant effects, Shortness of breath, respiratory arrest, narcosis, Dizziness, Nausea, agitation, spasms, inebriation, Headache, Stomach/intestinal disorders, ataxia (impaired locomotor coordination), cardiovascular disorders
Drying-out effect resulting in rough and chapped skin.

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

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to algae static test ErC50 - Chlamydomonas reinhardtii (green algae) - 13.3 mg/l - 72 h
Remarks: (ECHA)
The value is given in analogy to the following substances: Chloroform (Chloroform-D1-Deuteration)

Toxicity to bacteria Remarks: (ECHA)
The value is given in analogy to the following substances: Chloroform (Chloroform-D1-Deuteration)

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) semi-static test NOEC - Daphnia magna (Water flea) - 6.3 mg/l - 21 d
Remarks: (ECHA)
The value is given in analogy to the following substances: Chloroform

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 14 d
Result: 0 % - Not readily biodegradable.
(OECD Test Guideline 301C)

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 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: 1888 Class: 6.1 Packing group: III
Proper shipping name: Chloroform
Reportable Quantity (RQ): 10 lbs
Reportable Quantity (RQ): 10 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 1888 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: CHLOROFORM

IATA

UN number: 1888 Class: 6.1 Packing group: III
Proper shipping name: Chloroform

SECTION 15: Regulatory information

CERCLA Reportable Quantity

| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|---------------------------|----------|--------------------|-----------------------------|
| Chloroform-D1-Deuteration | 865-49-6 | 10 | 10 |
| Chloroform-D1-Deuteration | 865-49-6 | 10 | 10 (D022) |

SARA 304 Extremely Hazardous Substances Reportable Quantity

| Components | CAS-No. | Component RQ (lbs) | Calculated product RQ (lbs) |
|---------------------------|----------|--------------------|-----------------------------|
| Chloroform-D1-Deuteration | 865-49-6 | 10 | 10 |

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

| Components | CAS-No. | Component TPQ (lbs) |
|------------|---------|---------------------|
|------------|---------|---------------------|

| | | |
|---------------------------|----------|-------|
| Chloroform-D1-Deuteration | 865-49-6 | 10000 |
|---------------------------|----------|-------|

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

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

Chloroform- 865-49-6 >= 90 - <= 100 %
D1-Deuteration

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

The following chemical(s) are listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F):

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

This product contains the following toxic pollutants listed under the U.S. Clean Water Act Section 307

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

This product contains the following priority pollutants related to the U.S. Clean Water Act:

Chloroform-D1- 865-49-6 >= 90 - <= 100 %
Deuteration

US State Regulations

Massachusetts Right To Know

Chloroform-D1-Deuteration 865-49-6

Pennsylvania Right To Know

Chloroform-D1-Deuteration 865-49-6

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

California Prop. 65

WARNING: This product can expose you to chemicals including Chloroform-D1-Deuteration, which is/are known to the State of California to cause cancer and birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

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.

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