# SAFETY DATA SHEET

Version 8.10
Revision Date 08/10/2022
Print Date 10/30/2022

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Dichloroacetic acid for synthesis

Product Number : 8.03541
Catalogue No. : 803541
Brand : Millipore
Index-No. : 607-066-00-5
CAS-No. : 79-43-6

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Chemical for synthesis

### 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)**

Corrosive to Metals (Category 1), H290
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1), H314
Serious eye damage (Category 1), H318
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360
Effects on or via lactation, H362
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Specific target organ toxicity - repeated exposure, Oral (Category 2), Brain, Liver, Testes, H373
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 3), H412

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)

| | |
|---|---|
| H290 | May be corrosive to metals. |
| H311 | Toxic in contact with skin. |
| H314 | Causes severe skin burns and eye damage. |
| H335 | May cause respiratory irritation. |
| H351 | Suspected of causing cancer. |
| H360 | May damage fertility or the unborn child. |
| H362 | May cause harm to breast-fed children. |
| H373 | May cause damage to organs (Brain, Liver, Testes) through prolonged or repeated exposure if swallowed. |
| H400 | Very toxic to aquatic life. |
| H412 | Harmful 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. |
| P234 | Keep only in original container. |
| P260 | Do not breathe mist or vapors. |
| P263 | Avoid contact during pregnancy/ while nursing. |
| 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 + 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. |
| P390 | Absorb spillage to prevent material damage. |
| P391 | Collect spillage. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P405 | Store locked up. |
| P406 | Store in corrosive resistant container with a resistant inner liner. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Corrosive to the respiratory tract.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

| | | |
|---|---|---|
| Formula | : | C2H2Cl2O2 |
| Molecular weight | : | 128.94 g/mol |
| CAS-No. | : | 79-43-6 |
| EC-No. | : | 201-207-0 |
| Index-No. | : | 607-066-00-5 |

| Component | Classification | Concentration |
|---|---|---|
| **Dichloroacetic Acid** | | |
| | Met. Corr. 1; Acute Tox. 3; Skin Corr. 1A; Eye Dam. 1; Carc. 2; Repr. 1B; Lact. ; STOT RE 2; Aquatic Acute 1; H290, H311, H314, H318, H351, H360, H362, H373, H400<br>M-Factor - Aquatic Acute: 10 | <= 100 % |

| | | |
|---|---|---|
| **Trichloracetic acid** | | |
| | Skin Corr. 1A; Eye Dam. 1; STOT SE 3; Aquatic Acute 1; Aquatic Chronic 1; H314, H318, H335, H400, H410<br>Concentration limits:<br>>= 1 %: STOT SE 3, H335; | >= 1 - < 5 % |

| | | |
|---|---|---|
| **chloroacetic acid** | | |
| | Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; STOT SE 3; Aquatic Acute 1; H301, H331, H311, H314, H318, H335, H400<br>Concentration limits:<br>>= 5 %: STOT SE 3, H335;<br>M-Factor - Aquatic Acute: 10 | >= 0.1 - < 1 % |

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. Call in physician.

**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**
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Pulmonary failure possible after aspiration of vomit. Call a physician immediately. 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**
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
Combustible.
Fire may cause evolution of:
Hydrogen chloride gas
Phosgene
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
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**
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**
No metal or light-weight-metal containers. No metal containers.
Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

**Storage class**
Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which 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 |
|---|---|---|---|---|
| Dichloroacetic Acid | 79-43-6 | TWA | 0.5 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Confirmed animal carcinogen with unknown relevance to humans<br>Danger of cutaneous absorption | | |
| Trichloracetic acid | 76-03-9 | TWA | 0.5 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Confirmed animal carcinogen with unknown relevance to humans | | |
| | | TWA | 1 ppm<br>7 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | PEL | 1 ppm<br>5 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| chloroacetic acid | 79-11-8 | TWA | 0.5 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Not classifiable as a human carcinogen<br>Danger of cutaneous absorption | | |
| | | TWA | 0.5 ppm | USA. Workplace Environmental Exposure Levels (WEEL) |
| | | Skin | | |

## 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 EN374 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Splash contact

Material: Chloroprene
Minimum layer thickness: 0.65 mm
Break through time: 120 min
Material tested:KCL 720 Camapren®

**Body Protection**
Acid-resistant protective clothing

**Respiratory protection**
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<br>Color: colorless |
| b) | Odor | pungent |
| c) | Odor Threshold | No data available |
| d) | pH | 1.2 at 129 g/l at 20 °C (68 °F) |
| e) | Melting point/freezing point | Melting point/range: 13.5 °C (56.3 °F) |
| f) | Initial boiling point and boiling range | 193 - 195 °C 379 - 383 °F at 1,013.25 hPa |
| g) | Flash point | 113 °C (235 °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 | 0.19 hPa at 20 °C (68 °F) |
| l) | Vapor density | 4.45 - (Air = 1.0) |
| m) | Density | 1.567 g/cm3 at 20 °C (68 °F) |
| | Relative density | 1.5620 °C |
| n) | Water solubility | soluble |
| o) | Partition coefficient: n-octanol/water | log Pow: 0.92 - (Lit.), Bioaccumulation is not expected. |
| p) | Autoignition temperature | No data available |
| q) | Decomposition temperature | No data available |

| | | |
|---|---|---|
| r) | Viscosity | 4.696 mm2/s at 20 °C (68 °F) - 2.716 mm2/s at 40 °C (104 °F) - |
| s) | Explosive properties | No data available |
| t) | Oxidizing properties | none |

### 9.2 Other safety information

| | |
|---|---|
| Relative vapor density | 4.45 - (Air = 1.0) |

## 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.

### 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:
furfuryl alcohol
Violent reactions possible with:
Amines
Bases
Strong oxidizing agents
strong reducing agents
Sulfur compounds
Risk of ignition or formation of inflammable gases or vapours with:
Metals
mercaptans
Exothermic reaction with:
Water

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

Gives off hydrogen by reaction with metals.

### 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 - 2,684 mg/kg
(Calculation method)
LD50 Oral - Rat - 2,820 mg/kg (Dichloroacetic Acid)
(OECD Test Guideline 401)
Acute toxicity estimate Inhalation - 4 h - > 200 mg/l - dust/mist(Calculation method)

Inhalation: No data available
Inhalation: Corrosive to respiratory system. (Dichloroacetic Acid)
Acute toxicity estimate Dermal - 808.95 mg/kg
(Calculation method)
LD50 Dermal - Rabbit - 797 mg/kg (Dichloroacetic Acid)
Remarks: (ECHA)

**Skin corrosion/irritation**
Skin - Rabbit (Dichloroacetic Acid)
Result: Causes severe burns.
Remarks: (RTECS)

**Serious eye damage/eye irritation**
Eyes - Rabbit (Dichloroacetic Acid)
Result: Causes serious eye damage.
Remarks: (RTECS)
Causes serious eye damage. (Dichloroacetic Acid)

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
Test Type: In vitro mammalian cell gene mutation test
(Dichloroacetic Acid)
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative
Test Type: Ames test
(Dichloroacetic Acid)
Test system: Escherichia coli/Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: Chromosome aberration test in vitro
(Dichloroacetic Acid)
Test system: Chinese hamster ovary cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative
(Dichloroacetic Acid)
Test Type: Transgenic rodent somatic cell gene mutation assay
Species: Mouse
Cell type: Liver cells
Application Route: Oral

Result: negative
Remarks: (ECHA)
(Dichloroacetic Acid)
Test Type: Micronucleus test
Species: Rat
Cell type: Bone marrow
Application Route: Oral
Method: OECD Test Guideline 475
Result: negative

**Carcinogenicity**
Suspected of causing cancer. (Dichloroacetic Acid)

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Dichloroacetic Acid)

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**
May damage the unborn child. (Dichloroacetic Acid)
May damage fertility. Studies indicating a hazard to babies during the lactation period (Dichloroacetic Acid)

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
Oral - May cause damage to organs through prolonged or repeated exposure. - Brain, Liver, Testes

**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., Cough, Shortness of breath, Headache, Nausea (Dichloroacetic Acid)
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Dichloroacetic Acid)

## SECTION 12: Ecological information

### 12.1 Toxicity

No data available

| | |
|---|---|
| Toxicity to daphnia and other aquatic invertebrates | EC50 - Daphnia magna (Water flea) - 106 mg/l - 24 h<br>(Dichloroacetic Acid)<br>Remarks: (ECOTOX Database) |

### 12.2 Persistence and degradability

| | |
|---|---|
| Biodegradability | aerobic - Exposure time 15 d (Dichloroacetic Acid)<br>Result: 93 % - Readily biodegradable.<br>(OECD Test Guideline 301F) |

### 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
Forms corrosive mixtures with water even if diluted.
Discharge into the environment must be avoided.
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic to aquatic life.

## 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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

## SECTION 14: Transport information

**DOT (US)**
UN number: 1764 Class: 8 Packing group: II
Proper shipping name: Dichloroacetic acid
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

**IMDG**
UN number: 1764 Class: 8 Packing group: II EMS-No: F-A, S-B
Proper shipping name: DICHLOROACETIC ACID
Marine pollutant : yes

**IATA**
UN number: 1764 Class: 8 Packing group: II
Proper shipping name: Dichloroacetic acid

## SECTION 15: Regulatory information

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

## 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.


The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 8.10 Revision Date: 08/10/2022 Print Date: 10/30/2022