

SAFETY DATA SHEET

Version 6.3
Revision Date 04/14/2022
Print Date 06/01/2022

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

Product name : 4-Hydroxy-2,5-dimethyl-3(2H)-furanone

Product Number : W317410
Brand : Aldrich
CAS-No. : 3658-77-3

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)**

Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Skin sensitization (Category 1), H317

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)
H314 : Causes severe skin burns and eye damage.

H317	May cause an allergic skin reaction.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P272	Contaminated work clothing must not be allowed out of the workplace.
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.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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

3.2 Mixtures

Formula : C₆H₈O₃
Molecular weight : 128.13 g/mol

Component	Classification	Concentration
1,2-propanediol		
CAS-No. 57-55-6 EC-No. 200-338-0 Registration number 01-2119456809-23-XXXX		>= 70 - < 90 %
4-hydroxy-2,5-dimethylfuran-2(3H)-one		
CAS-No. 3658-77-3 EC-No. 222-908-8	Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1; H302, H314, H318, H317	>= 10 - < 20 %

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). 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

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

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 with liquid-absorbent material (e.g. Chemisorb®). 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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

hygroscopic Air sensitive.

Storage class

Storage class (TRGS 510): 8A: Combustible, corrosive 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
1,2-propanediol	57-55-6	TWA	10 mg/m ³	USA. Workplace Environmental Exposure Levels (WEEL)

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

required

Body Protection

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
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	215.5 °C 419.9 °F
g) Flash point	99 °C (210 °F)
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	1.057 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 | Not classified as explosive. |
| 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.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute toxicity estimate Dermal - 2,941 mg/kg
(Calculation method)

Skin corrosion/irritation

Mixture causes burns.

Serious eye damage/eye irritation

Mixture causes serious eye damage. Risk of blindness!

Aldrich - W317410

Page 6 of 11

Respiratory or skin sensitization

Mixture may cause an allergic skin reaction.

Germ cell mutagenicity

No data available

Carcinogenicity

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

No data available

Aspiration hazard

No data available

11.2 Additional Information

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

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components**1,2-propanediol****Acute toxicity**

LD50 Oral - Rat - male and female - 22,000 mg/kg

Remarks: (ECHA)

Inhalation: No data available

LD50 Dermal - Rabbit - > 2,000 mg/kg

Remarks: (ECHA)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Result: negative

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Remarks: (ECHA)

Species: Mouse - male - Bone marrow

Result: negative

Remarks: (ECHA)

Species: Rat - male - Bone marrow

Result: negative

Remarks: (ECHA)

Species: Rat - male

Result: negative

Remarks: (ECHA)

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard

No data available

4-hydroxy-2,5-dimethylfuran-2(3H)-one

Acute toxicity

LD50 Oral - Mouse - 1,608 mg/kg

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE)

Result: Corrosive

(OECD Test Guideline 431)

Serious eye damage/eye irritation

Eyes - chicken

Result: Causes serious eye damage.

(OECD Test Guideline 438)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Red blood cells (erythrocytes)

Result: positive

Species: Rat - male and female

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

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

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

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

Components

1,2-propanediol

Toxicity to fish

static test LC50 - Oncorhynchus mykiss (rainbow trout) -

Aldrich - W317410

40,613 mg/l - 96 h
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates static test LC50 - Ceriodaphnia dubia (water flea) - 18,340 mg/l - 48 h
(US-EPA)

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 19,000 mg/l - 96 h
(OECD Test Guideline 201)

Toxicity to bacteria NOEC - Pseudomonas putida - > 20,000 mg/l - 18 h
Remarks: (ECHA)

4-hydroxy-2,5-dimethylfuran-2(3H)-one

No data available

Toxicity to daphnia and other aquatic invertebrates static test - Daphnia magna (Water flea) - 6.8 mg/l - 48 h
(OECD Test Guideline 202)

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: 3267 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, basic, organic, n.o.s. (4-hydroxy-2,5-dimethylfuran-2(3H)-one)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 3267 Class: 8 Packing group: II EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, BASIC, ORGANIC, N.O.S. (4-hydroxy-2,5-dimethylfuran-2(3H)-one)

IATA

UN number: 3267 Class: 8 Packing group: II
Proper shipping name: Corrosive liquid, basic, organic, n.o.s. (4-hydroxy-2,5-dimethylfuran-2(3H)-one)

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.

SARA 311/312 Hazards

Acute Health Hazard

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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: 6.3

Revision Date: 04/14/2022

Print Date: 06/01/2022