SAFETY DATA SHEET

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

1.1 Product identifiers
Product name: α-Angelica lactone
Product Number: W329304
Brand: Aldrich
CAS-No.: 591-12-8

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)
Flammable liquids (Category 4), H227
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: Warning

Hazard statement(s)
H227: Combustible liquid.
H317: May cause an allergic skin reaction.
Precautionary statement(s)

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P261 Avoid breathing mist or vapors.
P272 Contaminated work clothing must not be allowed out of the workplace.
P280 Wear protective gloves/ eye protection/ face protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
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

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>4-Hydroxy-3-pentenoic acid γ-lactone 5-Methyl-2(3H)-furanone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C5H6O2</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>98.10 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>591-12-8</td>
</tr>
<tr>
<td>EC-No.</td>
<td>209-701-8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-Methylfuran-2(3H)-one</td>
<td>Flam. Liq. 4; Skin Sens. 1; H227, H317</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air.

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. 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
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
Remove container from danger zone and cool with water. 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. 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 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 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.

**Storage stability**
Recommended storage temperature
2 - 8 °C
Handle and store under inert gas. Air-, heat-, and moisture-sensitive.

**Storage class**
Storage class (TRGS 510): 10: Combustible liquids

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**
Contains no substances with occupational exposure limit values.

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**
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: clear, liquid
   Color: light yellow
b) Odor
   No data available
c) Odor Threshold
   No data available
d) pH
   No data available
e) Melting point/freezing point
   Melting point/range: 13 - 17 °C (55 - 63 °F) - lit.
f) Initial boiling point and boiling range
   55 - 56 °C 131 - 133 °F at 16 hPa - lit.
g) Flash point
   68 °C (154 °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
   1.092 g/cm³ at 25 °C (77 °F) - lit.
   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
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
Violent reactions possible with:
Strong oxidizing agents

10.4 Conditions to avoid
Exposure to moisture. Heat.
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

Acute toxicity
LD50 Oral - Rat - 3,900 mg/kg
Behavioral:Somnolence (general depressed activity).
Lungs, Thorax, or Respiration:Dyspnea.
(RTECS)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
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
RTECS: LU5075000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity
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

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)
NA-Number: 1993   Class: NONE   Packing group: III
Proper shipping name: Combustible liquid, n.o.s. (5-Methylfuran-2(3H)-one)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
Not dangerous goods

IATA
Not dangerous goods

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
Fire 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.

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