

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Shikimic acid  
  
Product Number : S5375  
Brand : Sigma  
  
CAS-No. : 138-59-0

#### 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA  
  
Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

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

Serious eye damage (Category 1), H318

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)

H318

Causes serious eye damage.

Precautionary statement(s)

P280

Wear eye protection/ face protection.

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.

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

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : (3R,4S,5R)-(-)-3,4,5-Trihydroxy-1-cyclohexenecarboxylic acid

Formula : C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>  
Molecular weight : 174.15 g/mol  
CAS-No. : 138-59-0  
EC-No. : 205-334-2

#### Hazardous components

Component	Classification	Concentration
<b>(3R,4S,5R)-3,4,5-Trihydroxycyclohex-1-enecarboxylic acid</b>		
	Eye Dam. 1; H318	90 - 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. Continue rinsing eyes during transport to hospital.

#### If swallowed

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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

---

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

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.

### 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.

Hazardous components without workplace control parameters

### 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

Face shield and safety glasses 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.

##### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

##### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

##### 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 particle respirator type N100 (US) or type P3 (EN 143) 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

Do not let product enter drains.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid 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: 185 - 187 °C (365 - 369 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
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	No data available
l) Vapour density	No data available
m) Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
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

No data available

#### 10.5 Incompatible materials

Strong oxidizing agents

#### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

---

### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 423)

Inhalation: No data available

Dermal: No data available

LD50 Intraperitoneal - Mouse - 1,000 mg/kg

##### Skin corrosion/irritation

Skin - in vitro assay

Result: No skin irritation

(OECD Test Guideline 439)

##### Serious eye damage/eye irritation

Eyes - In vitro study

Result: Corrosive to eyes - 240 min

(OECD Test Guideline 437)

##### Respiratory or skin sensitisation

in vivo assay - Mouse

Does not cause skin sensitisation.

(OECD Test Guideline 429)

##### Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: negative

Mouse

Dominant lethal test

##### Carcinogenicity

Carcinogenicity - Mouse - Oral

Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Gastrointestinal: Tumors.

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

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.

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 identified as a carcinogen or potential carcinogen by OSHA.

##### 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: GW4600000

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

---

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

Toxicity to fish	flow-through test LC50 - <i>Cyprinus carpio</i> (Carp) - > 100 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	flow-through test EC50 - <i>Daphnia magna</i> (Water flea) - > 10 - 100 mg/l - 48 h (ISO 6341)
Toxicity to algae	static test EC50 - <i>Selenastrum capricornutum</i> (green algae) - > 100 mg/l - 72 h (ISO 8692)

### 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d  
Result: 80 % - Readily biodegradable.

### 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 Other adverse effects

No data available

---

## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

---

## 14. TRANSPORT INFORMATION

**DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

---

## 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

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.

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
(3R,4S,5R)-3,4,5-Trihydroxycyclohex-1-enecarboxylic acid	138-59-0	

	CAS-No.	Revision Date
(3R,4S,5R)-3,4,5-Trihydroxycyclohex-1-enecarboxylic acid	138-59-0	

### New Jersey Right To Know Components

	CAS-No.	Revision Date
(3R,4S,5R)-3,4,5-Trihydroxycyclohex-1-enecarboxylic acid	138-59-0	

### 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.

---

## 16. OTHER INFORMATION

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

Eye Dam.	Serious eye damage
H318	Causes serious eye damage.

### HMIS Rating

Health hazard:	3
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

### NFPA Rating

Health hazard:	3
Fire Hazard:	0
Reactivity Hazard:	0

### Further information

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

### Preparation Information

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

Version: 5.3

Revision Date: 04/26/2017

Print Date: 11/10/2018

