

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 1272/2008

### Section 1. Identification of the Substance/Mixture and of the Company/Undertaking

- 1.1 Product Code:** 25054  
**Product Name:** 5-Caffeoylquinic Acid  
**Synonyms:** (1R,3R,4S,5R)-3-[[[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propen-1-yl]oxy]-1,4,5-trihydroxy-cyclohexanecarboxylic acid; 5-O-Caffeoylquinic Acid; trans-5-O-Caffeoylquinic Acid; 5-CQA; Neochlorogenic Acid;
- 1.2 Relevant identified uses of the substance or mixture and uses advised against:**  
**Relevant identified uses:** For research use only, not for human or veterinary use.
- 1.3 Details of the Supplier of the Safety Data Sheet:**  
**Company Name:** Cayman Chemical Company  
1180 E. Ellsworth Rd.  
Ann Arbor, MI 48108  
**Web site address:** www.caymanchem.com  
**Information:** Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**  
**Emergency Contact:** CHEMTREC Within USA and Canada: +1 (800)424-9300  
CHEMTREC Outside USA and Canada: +1 (703)527-3887

### Section 2. Hazards Identification

- 2.1 Classification of the Substance or Mixture:**  
**Skin Corrosion/Irritation, Category 2**  
**Serious Eye Damage/Eye Irritation, Category 2**  
**Specific Target Organ Toxicity (single exposure), Category 3**

**2.2 Label Elements:**



**GHS Signal Word:** **Warning**

**GHS Hazard Phrases:**

H315: Causes skin irritation.

H319: Causes serious eye irritation.

H335: May cause respiratory irritation.

**GHS Precaution Phrases:**

P261: Avoid breathing {dust/fume/gas/mist/vapors/spray}.

P264: Wash {hands} thoroughly after handling.

P280: Wear {protective gloves/protective clothing/eye protection/face protection}.

**GHS Response Phrases:**

P302+352: IF ON SKIN: Wash with plenty of soap and water.

P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P312: Call a POISON CENTER or doctor/physician if you feel unwell.

P332+313: If skin irritation occurs, get medical advice/attention.

P337+313: If eye irritation persists, get medical advice/attention.

P362+364: Take off contaminated clothing and wash it before reuse.

**GHS Storage and Disposal Phrases:**

Please refer to Section 7 for Storage and Section 13 for Disposal information.

- 2.3 Adverse Human Health** Causes serious eye irritation.
- Effects and Symptoms:** Causes skin irritation.
- Material may be irritating to the mucous membranes and upper respiratory tract.
- May be harmful by inhalation, ingestion, or skin absorption.
- May cause respiratory system irritation.
- To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

### Section 3. Composition/Information on Ingredients

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
906-33-2 GU8479500	[1R-(1.alpha.,3.alpha.,4.alpha.,5b.)]-3-[[3-(3,4-Dihydroxyphenyl)-1-oxoallyl]oxy]-1,4,5-trihydroxycyclohexanecarboxylic acid	100.0 %	212-997-1 NA	Skin Corr. 2: H315 Eye Damage 2: H319 STOT (SE) 3: H335 H336

### Section 4. First Aid Measures

- 4.1 Description of First Aid Measures:**
- In Case of Inhalation:** Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.
- In Case of Skin Contact:** Immediately wash skin with soap and plenty of water for at least 15 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.
- In Case of Eye Contact:** Hold eyelids apart and flush eyes with plenty of water for at least 15 minutes. Have eyes examined and tested by medical personnel.
- In Case of Ingestion:** Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.

### Section 5. Fire Fighting Measures

- 5.1 Suitable Extinguishing Media:** Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray.
- Media:** Use water spray to cool fire-exposed containers.
- Unsuitable Extinguishing Media:** A solid water stream may be inefficient.
- 5.2 Flammable Properties and Hazards:** No data available.
- Hazards:** No data available.
- Flash Pt:** No data.
- Explosive Limits:** LEL: No data. UEL: No data.
- Autoignition Pt:** No data.
- 5.3 Fire Fighting Instructions:** As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.

### Section 6. Accidental Release Measures

- 6.1 Protective Precautions,** Avoid raising and breathing dust, and provide adequate ventilation.
- Protective Equipment and** As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator,
- Emergency Procedures:** and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
- 6.2 Environmental** Take steps to avoid release into the environment, if safe to do so.
- Precautions:**
- 6.3 Methods and Material For** Contain spill and collect, as appropriate.
- Containment and Cleaning** Transfer to a chemical waste container for disposal in accordance with local regulations.
- Up:**

### Section 7. Handling and Storage

- 7.1 Precautions To Be Taken** Avoid breathing dust/fume/gas/mist/vapours/spray.
- in Handling:** Avoid prolonged or repeated exposure.
- 7.2 Precautions To Be Taken** Keep container tightly closed.
- in Storing:** Store in accordance with information listed on the product insert.

### Section 8. Exposure Controls/Personal Protection

- 8.1 Exposure Parameters:**
- 8.2 Exposure Controls:**
- 8.2.1 Engineering Controls** Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
- (Ventilation etc.):**
- 8.2.2 Personal protection equipment:**
- Eye Protection:** Safety glasses
- Protective Gloves:** Compatible chemical-resistant gloves
- Other Protective Clothing:** Lab coat
- Respiratory Equipment** NIOSH approved respirator, as conditions warrant.
- (Specify Type):**
- Work/Hygienic/Maintenan** Do not take internally.
- ce Practices:** Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower.
- Wash thoroughly after handling.
- No data available.

### Section 9. Physical and Chemical Properties

- 9.1 Information on Basic Physical and Chemical Properties**
- Physical States:** ☐ Gas ☐ Liquid ☒ Solid
- Appearance and Odor:** A crystalline solid
- pH:** No data.
- Melting Point:** No data.
- Boiling Point:** No data.
- Flash Pt:** No data.
- Evaporation Rate:** No data.
- Flammability (solid, gas):** No data available.
- Explosive Limits:** LEL: No data. UEL: No data.
- Vapor Pressure (vs. Air or mm** No data.
- Hg):**
- Vapor Density (vs. Air = 1):** No data.

<b>Specific Gravity (Water = 1):</b>	No data.
<b>Solubility in Water:</b>	No data.
<b>Solubility Notes:</b>	~25 mg/ml in PBS (pH 7.2); ~50 mg/ml in EtOH & DMSO; ~71 mg/ml in DMF;
<b>Octanol/Water Partition</b>	No data.
<b>Coefficient:</b>	
<b>Autoignition Pt:</b>	No data.
<b>Decomposition Temperature:</b>	No data.
<b>Viscosity:</b>	No data.
<b>9.2 Other Information</b>	
<b>Percent Volatile:</b>	No data.
<b>Molecular Formula &amp; Weight:</b>	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub> 354.3

### Section 10. Stability and Reactivity

<b>10.1 Reactivity:</b>	No data available.
<b>10.2 Stability:</b>	Unstable [ ]      Stable [ X ]
<b>10.3 Stability Note(s):</b>	Stable if stored in accordance with information listed on the product insert.
<b>Polymerization:</b>	Will occur [ ]      Will not occur [ X ]
<b>10.4 Conditions To Avoid:</b>	No data available.
<b>10.5 Incompatibility - Materials</b>	strong oxidizing agents
<b>To Avoid:</b>	
<b>10.6 Hazardous</b>	carbon dioxide
<b>Decomposition or Byproducts:</b>	carbon monoxide

### Section 11. Toxicological Information

<b>11.1 Information on Toxicological Effects:</b>	The toxicological effects of this product have not been thoroughly studied.				
CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
906-33-2	[1R-(1.alpha.,3.alpha.,4.alpha.,5b.)]-3-[[3-(3,4-Dihydroxyphenyl)-1-oxoallyl]oxy]-1,4,5-trihydroxycyclohexanecarboxylic acid	n.a.	n.a.	n.a.	n.a.

### Section 12. Ecological Information

<b>12.1 Toxicity:</b>	Avoid release into the environment. Runoff from fire control or dilution water may cause pollution.
<b>12.2 Persistence and Degradability:</b>	No data available.
<b>12.3 Bioaccumulative Potential:</b>	No data available.
<b>12.4 Mobility in Soil:</b>	No data available.
<b>12.5 Results of PBT and vPvB assessment:</b>	No data available.
<b>12.6 Other adverse effects:</b>	No data available.

### Section 13. Disposal Considerations

**13.1 Waste Disposal Method:** Dispose in accordance with local, state, and federal regulations.

### Section 14. Transport Information

**14.1 LAND TRANSPORT (US DOT):**

**DOT Proper Shipping Name:** Not dangerous goods.

**DOT Hazard Class:**

**UN/NA Number:**

**14.1 LAND TRANSPORT (European ADR/RID):**

**ADR/RID Shipping Name:** Not dangerous goods.

**UN Number:**

**Hazard Class:**

**14.3 AIR TRANSPORT (ICAO/IATA):**

**ICAO/IATA Shipping Name:** Not dangerous goods.

**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.

### Section 15. Regulatory Information

**EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists**

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
906-33-2	[1R-(1.alpha.,3.alpha.,4.alpha.,5b.)]-3-[[3-(3,4-Dihydroxyphenyl)-1-oxoallyl]oxy]-1,4,5-trihydroxycyclohexanecarboxylic acid	No	No	No

  

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
906-33-2	[1R-(1.alpha.,3.alpha.,4.alpha.,5b.)]-3-[[3-(3,4-Dihydroxyphenyl)-1-oxoallyl]oxy]-1,4,5-trihydroxycyclohexanecarboxylic acid	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No

**Regulatory Information Statement:** This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.

### Section 16. Other Information

**Revision Date:** 07/09/2018

**Additional Information About This Product:** No data available.

**This Product:**

**Company Policy or Disclaimer:** DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.