

Punicalagin SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Punicalagin

* Catalog Number: S9131

* CAS Number: 65995-63-3

* IUPAC Name: D-Glucose, cyclic 4,6-[(2S,2'S)-2,2'-(5,10-dihydro-2,3,7,8-tetrahydroxy-5,10-dioxo[1]benzopyrano[5,4,3-cde][1]benzopyran-1,6-diyl)bis[3,4,5-trihydroxybenzoate]] cyclic 2,3-[(1S)-4,4',5,5',6,6'-hexahydroxy[1,1'-biphenyl]-2,2'-dicarboxylate]

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals

* TollFree: +1 877 796-6397

* Tel: +1 832 582-8158

* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Not classified as a hazardous substance according to GHS.

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s) None.

Signal Word Not applicable

Hazard statement(s) None.

Precautionary statement(s) None.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Punicalagin

CAS Number: 65995-63-3

PubChem CID: 16129719

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Wear self contained breathing apparatus for fire fighting if necessary.

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: Criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices.

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

Provide appropriate exhaust ventilation at places where dust is formed.

If pregnant, nursing or taking any medications, consult your healthcare professional before taking this product. Keep out of reach of children.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Keep container tightly closed in a dry and well-ventilated place. Moisture sensitive. Light sensitive. Store under inert gas. Keep in a dry place.

Refrigerate after opening. Consume within 60 days of opening.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Moisture sensitive. Light sensitive. Store under inert gas. Keep in a dry place.

Refrigerate after opening. Consume within 60 days of opening.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear safety glasses with side shields.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- a) Appearance: Yellow powder
- 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: 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) Vapor pressure: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: In methanol, 5 mg/mL, clear
- o) Partition coefficient: n-octanol/water: Log P: 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 information

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Air, light, and moisture sensitive.

Strong oxidizing agents, Acids

10.6 Hazardous decomposition products

No data available.

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION**11.1 Information on toxicological effects****Acute toxicity:**

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

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.

11.2 Additional information

No additional toxicological information available.

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

Punicalagin's production and use as an antineoplastic may result in its release to the environment through various waste streams. The compound is present in Punica granatum L., pomegranate. If released to air, an estimated vapor pressure of 3.5×10^{-61} mm Hg at 25 °C indicates punicalagin will exist solely in the particulate phase in the atmosphere. Particulate-phase punicalagin will be removed from the atmosphere by wet or dry deposition. Punicalagin contains chromophores that absorb at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, punicalagin is expected to have no mobility based upon an estimated Koc of $1 \times 10^{+10}$. Volatilization from moist soil surfaces is not expected to be an important fate process based upon

an estimated Henry's Law constant of 1.8×10^{-16} atm-cu m/mole. If released into water, punicalagin is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. Hydrolysis is expected to be an important environmental fate process since this compound contains functional groups that hydrolyze under environmental conditions. Occupational exposure to punicalagin may occur through dermal contact with this compound at workplaces where punicalagin is extracted.

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.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable.

15. REGULATORY INFORMATION

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

US EPA / TSCA: Not available in public databases.

EU ECHA / REACH: Not available in public databases.

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:

No SARA Hazards.

Massachusetts Right To Know Components:

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components:

No components are subject to the Pennsylvania Right to Know Act.

New Jersey Right To Know Components:

No components are subject to the New Jersey Right to Know Act.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/10

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.