

Safety Data Sheet acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

1 Identification

- **Product identifier**
- **Trade name: (S)-Equol**
- **Synonym**
 (S)-3,4-dihydro-3-(4-hydroxyphenyl)-2H-1-benzopyran-7-ol
 4',7-Dihydroxyisoflavan
 (-)-Equol
 4',7-Isosoflavandiol
- **Article number:** 10010173
- **CAS Number:**
531-95-3
- **EC number:**
208-522-2
- **Application of the substance / the mixture**
 This product is for research use - Not for human or veterinary diagnostic or therapeutic use. It is the responsibility of the purchaser to determine suitability for other applications.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
 Cayman Chemical Co.
 1180 E. Ellsworth Rd.
 Ann Arbor, MI 48108
 USA
- **Information department:** Product safety department
- **Emergency telephone number:**
 During normal opening times: +1 (734) 971-3335
 US/CANADA: 800-424-9300
 Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

- **Classification of the substance or mixture**
 The substance is not classified, according to the Globally Harmonized System (GHS).

- **Label elements**
- **GHS label elements** None
- **Hazard pictograms** None
- **Signal word** None
- **Hazard statements** None
- **Classification system:**
- **NFPA ratings (scale 0 - 4)**



- **HMIS-ratings (scale 0 - 4)**



(Contd. on page 2)

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 1)

- **Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.

3 Composition/information on ingredients

- **Chemical characterization: Substances**
- **CAS No. Description**
531-95-3 (S)-Equol
- **Identification number(s)**
- **EC number:** 208-522-2

4 First-aid measures

- **Description of first aid measures**
- **General information:** No special measures required.
- **After inhalation:** Supply fresh air; consult doctor in case of complaints.
- **After skin contact:** Generally the product does not irritate the skin.
- **After eye contact:** Rinse opened eye for several minutes under running water.
- **After swallowing:** If symptoms persist consult doctor.
- **Information for doctor:**
- **Most important symptoms and effects, both acute and delayed**
May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects.
No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
Use fire fighting measures that suit the environment.
A solid water stream may be inefficient.
- **Special hazards arising from the substance or mixture** No further relevant information available.
- **Advice for firefighters**
- **Protective equipment:** No special measures required.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures** Not required.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:** Pick up mechanically.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
- **Protective Action Criteria for Chemicals**
- **PAC-1:** Substance is not listed.

(Contd. on page 3)

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 2)

- **PAC-2:** Substance is not listed.
- **PAC-3:** Substance is not listed.

7 Handling and storage

- **Handling:**
- **Precautions for safe handling** No special measures required.
- **Information about protection against explosions and fires:** No special measures required.
- **Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** None.
- **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

- **Additional information about design of technical systems:** No further data; see item 7.
- **Control parameters**
- **Components with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Personal protective equipment:**
- **General protective and hygienic measures:**
The usual precautionary measures for handling chemicals should be followed.
- **Breathing equipment:** Not required.
- **Protection of hands:**
The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
- **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:** Not required.

9 Physical and chemical properties

- **Information on basic physical and chemical properties**
- **General Information**
- **Appearance:**
 - **Form:** Crystalline
 - **Color:** Not determined.
- **Odor:** Characteristic
- **Structural Formula** C₁₅H₁₄O₃

(Contd. on page 4)

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 3)

· Molecular Weight	242.3 g/mol
· Odor threshold:	Not determined.
· pH-value:	Not applicable.
· Change in condition	
Melting point/Melting range:	Undetermined.
Boiling point/Boiling range:	Undetermined.
· Flash point:	Not applicable.
· Flammability (solid, gaseous):	Product is not flammable.
· Decomposition temperature:	Not determined.
· Auto igniting:	Not determined.
· Danger of explosion:	Product does not present an explosion hazard.
· Explosion limits:	
Lower:	Not determined.
Upper:	Not determined.
· Vapor pressure:	Not applicable.
· Density:	Not determined.
· Relative density	Not determined.
· Vapor density	Not applicable.
· Evaporation rate	Not applicable.
· Solubility in / Miscibility with	
Water:	Not determined.
· Partition coefficient (n-octanol/water):	Not determined.
· Viscosity:	
Dynamic:	Not applicable.
Kinematic:	Not applicable.
SOLUBILITY	~0.1 mg/ml in a 1:10 solution of EtOH:PBS (pH 7.2); ~20 mg/ml in EtOH & DMSO; ~15 mg/ml in DMF
· Other information	No further relevant information available.

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong oxidizing agents
- **Hazardous decomposition products:** carbon oxides

11 Toxicological information

- **RTECS Number** DJ2887080

(Contd. on page 5)

US

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 4)

- **Information on toxicological effects**

- **Acute toxicity:**

- **LD/LC50 values that are relevant for classification:**

Oral	TDLO	525 mg/kg//3W (intermittent) (mouse)
	Subcutaneous TDLO	50 mg/kg (rat)
	Intraperitoneal TDLO	50 mg/kg (mouse)

- **Primary irritant effect:**

- **on the skin:** No irritant effect.

- **on the eye:** No irritating effect.

- **Sensitization:** No sensitizing effects known.

- **Additional toxicological information:**

When used and handled according to specifications, the product does not have any harmful effects according to our experience and the information provided to us.

The substance is not subject to classification.

- **Carcinogenic categories**

- **IARC (International Agency for Research on Cancer)** Substance is not listed.

- **NTP (National Toxicology Program)** Substance is not listed.

- **OSHA-Ca (Occupational Safety & Health Administration)** Substance is not listed.

12 Ecological information

- **Toxicity**

- **Aquatic toxicity:** No further relevant information available.

- **Persistence and degradability** No further relevant information available.

- **Behavior in environmental systems:**

- **Bioaccumulative potential** No further relevant information available.

- **Mobility in soil** No further relevant information available.

- **Additional ecological information:**

- **General notes:**

Water hazard class 1 (Self-assessment): slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

- **Results of PBT and vPvB assessment**

- **PBT:** Not applicable.

- **vPvB:** Not applicable.

- **Other adverse effects** No further relevant information available.

13 Disposal considerations

- **Waste treatment methods**

- **Recommendation:** Smaller quantities can be disposed of with household waste.

- **Uncleaned packagings:**

- **Recommendation:** Disposal must be made according to official regulations.

US

(Contd. on page 6)

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 5)

14 Transport information

· UN-Number	
· DOT, IMDG, IATA	not regulated
· UN proper shipping name	
· DOT, IMDG, IATA	not regulated
· Transport hazard class(es)	
· DOT, ADN, IMDG, IATA	
· Class	not regulated
· Packing group	
· DOT, IMDG, IATA	not regulated
· Environmental hazards:	Not applicable.
· Special precautions for user	Not applicable.
· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· UN "Model Regulation":	not regulated

15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.
- **Sara**
- **Section 355 (extremely hazardous substances):** Substance is not listed.
- **Section 313 (Specific toxic chemical listings):** Substance is not listed.
- **TSCA (Toxic Substances Control Act):** Substance is not listed.
- **Hazardous Air Pollutants** Substance is not listed.
- **Proposition 65**
- **Chemicals known to cause cancer:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for females:** Substance is not listed.
- **Chemicals known to cause reproductive toxicity for males:** Substance is not listed.
- **Chemicals known to cause developmental toxicity:** Substance is not listed.
- **Carcinogenic categories**
- **EPA (Environmental Protection Agency)** Substance is not listed.
- **TLV (Threshold Limit Value)** Substance is not listed.
- **NIOSH-Ca (National Institute for Occupational Safety and Health)** Substance is not listed.
- **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

(Contd. on page 7)

Safety Data Sheet

acc. to OSHA HCS

Printing date 06/12/2021

Revision date 06/12/2021

Trade name: (S)-Equol

(Contd. from page 6)

· **Department issuing SDS:** Environment protection department.

· **Contact:** -

· **Date of preparation / last revision** 06/12/2021 / -

· **Abbreviations and acronyms:**

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

US