

(S)-Equol

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830
Date of issue: 3/4/2019 Version: 1.0

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

1.1. Product identifier

Product form	: Substance
Substance name	: (S)-Equol
IUPAC name	: (3S)-3-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-ol
EC-No.	: 208-522-2
CAS-No.	: 531-95-3
Product code	: 89989072
Formula	: C ₁₅ H ₁₄ O ₃
Product group	: Raw material

1.2. Relevant identified uses of the substance or mixture and uses advised against

1.2.1. Relevant identified uses

Main use category	: Laboratory use, Industrial use, Professional use
Industrial/Professional use spec	: For professional use only

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Safell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Not classified

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Not classified.

2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%
(S)-Equol	(CAS-No.) 531-95-3 (EC-No.) 208-522-2	100

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: If possible show this sheet, if not available show packaging or label. If you feel unwell, seek medical advice. Do not leave affected person unattended.
First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing.
First-aid measures after skin contact	: If skin irritation or rash occurs: Rinse skin with water/shower. Do not remove clothing if it sticks to the skin.
First-aid measures after eye contact	: Rinse eyes with water as a precaution. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.

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First-aid measures after ingestion : Rinse mouth out with water. Do not induce vomiting. Do not give an unconscious person anything to drink.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects : Not expected to present a significant hazard under anticipated conditions of normal use.

Symptoms/effects after inhalation : Dust of the product, if present, may cause respiratory irritation after an excessive inhalation exposure.

Symptoms/effects after skin contact : Dust may cause irritation in skin folds or by contact in combination with tight clothing.

Symptoms/effects after eye contact : Dust from this product may cause eye irritation. redness, itching, tears.

Symptoms/effects after ingestion : May cause irritation to the digestive tract.

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Foam. Dry powder. Carbon dioxide. Water spray. Sand.

Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂).

5.3. Advice for firefighters

Precautionary measures fire : Keep container tightly closed and away from heat, sparks and flame. Exposure to fire/heat: seal off low-lying areas.

Firefighting instructions : Do not enter fire area without proper protective equipment, including respiratory protection. Evacuate area. Use water spray or fog for cooling exposed containers. Use extinguishing agent suitable for surrounding fire.

Protection during firefighting : Use self-contained breathing apparatus and chemically protective clothing.

Other information : Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : No flames, no sparks. Eliminate all sources of ignition. Isolate from fire, if possible, without unnecessary risk. Avoid dust formation.

6.1.1. For non-emergency personnel

Protective equipment : Wear recommended personal protective equipment.

Emergency procedures : Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Avoid contact with skin, eyes and clothing. Do not touch or walk on the spilled product.

Measures in case of dust release : Keep upwind. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc).

6.1.2. For emergency responders

Protective equipment : Use self-contained breathing apparatus and chemically protective clothing.

Emergency procedures : Stop release. Prevent from entering sewers, basements and workpits, or any place where its accumulation can be dangerous.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : On land, sweep or shovel into suitable containers. Minimise generation of dust. Store away from other materials.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Does not present any particular risk, provided it is handled in accordance with good occupational hygiene and safety practice and that precautions are taken to avoid the inhalation of dust. Ensure good ventilation of the work station. Do not handle until all safety precautions have been read and understood.

Hygiene measures : Take off immediately all contaminated clothing and wash it before reuse. Contaminated work clothing should not be allowed out of the workplace. Do not eat, drink or smoke when using this product. Always wash hands after handling the product. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ensure adequate ventilation, especially in confined areas.

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Storage conditions	: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Incompatible products	: Strong oxidisers.
Incompatible materials	: Refer to Section 10 on Incompatible Materials.
Storage area	: Keep frozen. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Ensure exposure is below occupational exposure limits (where available). Ensure that there is a suitable ventilation system. Handle in accordance with good industrial hygiene and safety procedures.

Personal protective equipment:

Avoid all unnecessary exposure. Wear recommended personal protective equipment.

Hand protection:

The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374. Always wash hands after handling the product

Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Nitrile rubber (NBR)	6 (> 480 minutes)	0.11		EN 374

Eye protection:

Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against powders and dusts.

Type	Use	Characteristics	Standard
Safety glasses	Dust	With side shields	EN 166

Skin and body protection:

Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use. Wash all protective clothing after use

Type	Standard
Long sleeved protective clothing	EN ISO 13982

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment. No respiratory protection needed under normal use conditions

Device	Filter type	Condition	Standard
Dust mask	Type P1	Dust protection	EN 14387

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Molecular mass	: 242.27 g/mol
Colour	: white.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available

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Flammability (solid, gas)	: Non flammable.
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: No data available
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under recommended handling and storage conditions (see section 7).

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

10.5. Incompatible materials

Strong oxidizers.

10.6. Hazardous decomposition products

No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO₂).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified
Skin corrosion/irritation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity	: Not classified
Chronic aquatic toxicity	: Not classified

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12.2. Persistence and degradability

(S)-Equol (531-95-3)

Persistence and degradability	No data available.
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12.3. Bioaccumulative potential

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Bioaccumulative potential	No data available.
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12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

(S)-Equol (531-95-3)

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

12.6. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.2. UN proper shipping name				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.3. Transport hazard class(es)				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.4. Packing group				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.5. Environmental hazards				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
No supplementary information available				

14.6. Special precautions for user

Overland transport

Not regulated

Transport by sea

Not regulated

Air transport

Not regulated

Inland waterway transport

Not regulated

Rail transport

Not regulated

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

SECTION 15: Regulatory information

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

15.1.1. EU-Regulations

No REACH Annex XVII restrictions

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(S)-Equol is not on the REACH Candidate List

(S)-Equol is not on the REACH Annex XIV List

Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations

Germany

12th Ordinance Implementing the Federal Immission Control Act - 12.BImSchV : Is not subject of the 12. BImSchV (Hazardous Incident Ordinance)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed

SZW-lijst van mutagene stoffen : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Borstvoeding : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Vruchtbaarheid : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Ontwikkeling : The substance is not listed

15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product