Sulisobenzone SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Sulisobenzone
* Catalog Number: S4652
* CAS Number: 4065-45-6
* IUPAC Name: Benzenesulfonic acid, 5-benzoyl-4-hydroxy-2-methoxy-

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):

Skin irritation: Category 2. H315

Skin sensitization: Category 1. H317

Serious eye damage: Category 1. H318

Serious eye irritation: Category 2. H319

Specific target organ toxicity (single exposure): Category 3. H335

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)	
Signal Word	Danger
Hazard statement(s)	H315: Causes skin irritation H317: May cause an allergic skin reaction H318: Causes serious eye damage H319: Causes serious eye irritation H335: May cause respiratory irritation
Precautionary statement(s)	None.

Prevention	P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264: Wash hands thoroughly after handling. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P271: Use only outdoors or in a well-ventilated area. P272: Contaminated work clothing should not be allowed out of the workplace. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P305+P354: IF IN EYES: Immediately rinse with water for several minutes. P317: Get emergency medical help. P319: Get medical help if you feel unwell. P321: Specific treatment (see information on this label and safety datasheet)). P332+P317: If skin irritation occurs: Get medical help. P333+P317: If skin irritation or rash occurs: Get medical help. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P362+P364: Take off contaminated clothing and wash it before reuse.
Storage	P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Sulisobenzone

CAS Number: 4065-45-6

PubChem CID: 19988

Molecular formula: C14H12O6S

Molecular weight: 308.31 g/mol

IUPAC name: 5-benzoyl-4-hydroxy-2-methoxybenzenesulfonic acid

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

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

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. Do not let product enter drains. Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components

tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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.

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

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

Store below 40 °C (104 °F), preferably between 15 and 30 deg. C (59 and 86 deg. F), unless otherwise specified by manufacturer. /Sunscreen agents, topical/

7.2 Conditions for safe storage, including any incompatibilities

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

Store below 40 °C (104 °F), preferably between 15 and 30 deg. C (59 and 86 deg. F), unless otherwise specified by manufacturer. /Sunscreen agents, topical/

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 only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles and face shield.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Light tan solid; [Merck Index]

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 145 °C

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 water, 2.5X10+5 mg/L at 25 °C

o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 2.2

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

Topological Polar Surface Area (TPSA): 109 Å²

Complexity: 462

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.

Avoid strong oxidizing agents, strong acids, and strong bases.

10.5 Incompatible materials

Strong oxidizing agents.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO□), Sulfur oxides (SOx).

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:

Causes skin irritation (H315).

Serious eye damage/eye irritation:

Causes serious eye damage (H318).

Respiratory or skin sensitization:

May cause an allergic skin reaction (H317).

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

/AQUATIC SPECIES/ In this work, /the authors/ evaluate whether in vitro systems are good predictors for in vivo estrogenic activity in fish. /Investigators/ focus on UV filters being used in sunscreens and in UV stabilization of materials. First, /investigators/ determined the estrogenic activity of 23 UV filters and one UV filter metabolite employing a recombinant yeast carrying the estrogen receptor of rainbow trout (rtERalpha) and made comparisons with yeast carrying the human hERalpha for receptor specificity. Benzophenone-1 (BP1), benzophenone-2 (BP2), 4,4-dihydroxybenzophenone, 4-hydroxybenzophenone, 2,4,4-trihydroxy-benzophenone, and phenylsalicylate showed full dose-response curves with maximal responses of 81-115%, whereas 3-benzylidene camphor (3BC), octylsalicylate, benzylsalicylate, benzophenone-3, and benzophenone-4 displayed lower maximal responses of 15-74%. Whereas the activity of 17beta-estradiol was lower in the rtERalpha than the hERalpha assay, the activities

of UV filters were similar or relatively higher in rtERalpha, indicating different relative binding activities of both ER. Subsequently, /investigators/ analyzed whether the in vitro estrogenicity of eight UV filters is also displayed in vivo in fathead minnows by the induction potential of vitellogenin after 14 days of aqueous exposure. Of the three active compounds in vivo, 3BC induced vitellogenin at lower concentrations (435 ug/L) than BP1 (4919 ug/L) and BP2 (8783 ug/L). The study shows, for the

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 2.2

Low potential for bioaccumulation (Log P < 3).

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: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

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 (short-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

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.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: Benzenesulfonic acid, 5-benzoyl-4-hydroxy-2-methoxy-

- FDA Requirements: Sunscreen active ingredients. The active ingredient of the product consists of any of the following, within the concentration specified for each ingredient, and the finished product provides a minimum SPF value of not less than 2 as measured by the testing procedures established in subpart D of thi

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: 2026/09/09

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.