

## SAFETY DATA SHEET

Version 6.1  
Revision Date 05/28/2017  
Print Date 11/18/2018

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : 6,8-Bis(benzylthio)-octanoic acid

Product Number : SML0404

Brand : Sigma

CAS-No. : 95809-78-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

#### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 Spruce Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

##### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

#### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word : Warning

Hazard statement(s)

H410 : Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P273 : Avoid release to the environment.

P391 : Collect spillage.

P501 : Dispose of contents/ container to an approved waste disposal plant.

#### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : CPI 613  
6,8-Bis[(phenylmethyl)thio]octanoic acid

Formula : C<sub>22</sub>H<sub>28</sub>O<sub>2</sub>S<sub>2</sub>

Molecular weight : 388.59 g/mol

CAS-No. : 95809-78-2

No components need to be disclosed according to the applicable regulations.

For the full text of the H-Statements mentioned in this Section, see Section 16.

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### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

##### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

##### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

##### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

##### In case of eye contact

Flush eyes with water as a precaution.

##### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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### 5. FIREFIGHTING MEASURES

#### 5.1 Extinguishing media

##### Suitable extinguishing media

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

#### 5.2 Special hazards arising from the substance or mixture

Carbon oxides, Sulphur oxides

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

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### 6. ACCIDENTAL RELEASE MEASURES

#### 6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.

For personal protection see section 8.

#### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

#### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

#### 6.4 Reference to other sections

For disposal see section 13.

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### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature 2 - 8 °C

#### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

##### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

#### 8.2 Exposure controls

##### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

##### Personal protective equipment

###### Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

###### Skin protection

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.

###### Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

###### Respiratory protection

Respiratory protection is not required. Where protection from nuisance level (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

###### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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### 9. PHYSICAL AND CHEMICAL PROPERTIES

#### 9.1 Information on basic physical and chemical properties

- |  |                           |
|--|---------------------------|
| a) Appearance                              | Form: solid               |
| b) Odour                                   | No data available         |
| c) Odour Threshold                         | No data available         |
| d) pH                                      | No data available         |
| e) Melting point/freezing point            | 66 - 67 °C (151 - 153 °F) |
| f) Initial boiling point and boiling range | No data available         |
| g) Flash point                             | ( )Not applicable         |

h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	No data available
l)	Vapour density	No data available
m)	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	log Pow: 6.189
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 safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulphur oxides  
In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available 6,8-bis(Benzylthio)-octanoic acid  
Inhalation: No data available (6,8-bis(Benzylthio)-octanoic acid)  
Dermal: No data available (6,8-bis(Benzylthio)-octanoic acid)  
No data available (6,8-bis(Benzylthio)-octanoic acid)

#### Skin corrosion/irritation

No data available (6,8-bis(Benzylthio)-octanoic acid)

#### Serious eye damage/eye irritation

No data available (6,8-bis(Benzylthio)-octanoic acid)

**Respiratory or skin sensitisation**

No data available(6,8-bis(Benzylthio)-octanoic acid)

**Germ cell mutagenicity**

No data available(6,8-bis(Benzylthio)-octanoic acid)

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available(6,8-bis(Benzylthio)-octanoic acid)

No data available(6,8-bis(Benzylthio)-octanoic acid)

**Specific target organ toxicity - single exposure**

No data available(6,8-bis(Benzylthio)-octanoic acid)

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available(6,8-bis(Benzylthio)-octanoic acid)

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.(6,8-bis(Benzylthio)-octanoic acid)

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available(6,8-bis(Benzylthio)-octanoic acid)

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Very toxic to aquatic life with long lasting effects.

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

Not dangerous goods

### IMDG

UN number: 3077 Class: 9

Packing group: III

EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (6,8-bis(Benzylthio)-octanoic acid

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Marine pollutant : yes

### IATA

UN number: 3077 Class: 9

Packing group: III

Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (6,8-bis(Benzylthio)-octanoic acid

)

### Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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## 15. REGULATORY INFORMATION

### 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

6,8-bis(Benzylthio)-octanoic acid	CAS-No. 95809-78-2	Revision Date
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### New Jersey Right To Know Components

6,8-bis(Benzylthio)-octanoic acid	CAS-No. 95809-78-2	Revision Date
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### California Prop. 65 Components

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

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

**HMIS Rating**

Health hazard:	0
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

**NFPA Rating**

Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	0

**Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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