

## SAFETY DATA SHEET

Version 5.3  
Revision Date 10/21/2016  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide

Product Number : A9013  
Brand : Sigma

CAS-No. : 402-40-4

## 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

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

Acute toxicity, Oral (Category 2), H300  
Acute toxicity, Inhalation (Category 1), H330  
Acute toxicity, Dermal (Category 2), H310

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 : Danger

Hazard statement(s)  
H300 + H310 + H330 : Fatal if swallowed, in contact with skin or if inhaled

Precautionary statement(s)  
P260 : Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.  
P262 : Do not get in eyes, on skin, or on clothing.  
P264 : Wash skin thoroughly after handling.  
P270 : Do not eat, drink or smoke when using this product.  
P271 : Use only outdoors or in a well-ventilated area.  
P280 : Wear protective gloves/ protective clothing.  
P284 : Wear respiratory protection.  
P301 + P310 : IF SWALLOWED: Immediately call a POISON CENTER/doctor.

|             |                                                                                                  |
|-------------|--------------------------------------------------------------------------------------------------|
| P302 + P350 | IF ON SKIN: Gently wash with plenty of soap and water.                                           |
| P304 + P340 | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. |
| P310        | Immediately call a POISON CENTER/doctor.                                                         |
| P320        | Specific treatment is urgent (see supplemental first aid instructions on this label).            |
| P330        | Rinse mouth.                                                                                     |
| P361        | Remove/Take off immediately all contaminated clothing.                                           |
| P363        | Wash contaminated clothing before reuse.                                                         |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed.                                 |
| P405        | Store locked up.                                                                                 |
| P501        | Dispose of contents/ container to an approved waste disposal plant.                              |

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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |                                                                    |
|------------------|--------------------------------------------------------------------|
| Synonyms         | : BW 284c51                                                        |
| Formula          | : C <sub>27</sub> H <sub>38</sub> Br <sub>2</sub> N <sub>2</sub> O |
| Molecular weight | : 566.41 g/mol                                                     |
| CAS-No.          | : 402-40-4                                                         |

#### Hazardous components

| Component                                                           | Classification                                                     | Concentration |
|---------------------------------------------------------------------|--------------------------------------------------------------------|---------------|
| <b>1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide</b> |                                                                    |               |
|                                                                     | Acute Tox. 2; Acute Tox. 1;<br>Acute Tox. 2; H300 + H310 +<br>H330 | <= 100 %      |

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

## 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. Move out of dangerous area.

#### 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. Take victim immediately to hospital. 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

## 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**

No data available

## **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**

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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.

## **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**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

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.

## **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**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

### **Personal protective equipment**

#### **Eye/face protection**

Face shield and safety glasses 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.

#### **Full contact**

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

#### **Splash contact**

Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### **Body Protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### **Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. 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.

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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                 | 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) 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       | 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 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, Nitrogen oxides (NO<sub>x</sub>), Hydrogen bromide gas

Other decomposition products - No data available

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

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### 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

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

**Additional Information**

RTECS: Not available

Cholinesterase inhibitor

Cholinesterase inhibitors can cause heavy salivation and secretion in the lungs, lachrymation, blurred vision, involuntary defecation, diarrhea, tremor, ataxia, sweating, hypothermia, lowered heart rate, and/or a fall in blood pressure as a result of their action at cholinergic nerve sites., Headache, Nausea, Vomiting, Dizziness, Drowsiness, Confusion., Weakness, Muscle cramps/spasms., Change in pupil size., Fever, Seizures., Incoordination.

Stomach - Irregularities - Based on Human Evidence

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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

**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**

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. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

UN number: 2811

Class: 6.1

Packing group: I

Proper shipping name: Toxic solids, organic, n.o.s. (1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide)

Poison Inhalation Hazard: No

**IMDG**

UN number: 2811

Class: 6.1

Packing group: I

EMS-No: F-A, S-A

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide)

**IATA**

UN number: 2811

Class: 6.1

Packing group: I

Proper shipping name: Toxic solid, organic, n.o.s. (1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide)

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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

Acute Health Hazard, Chronic Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

|                                                              | CAS-No.  | Revision Date |
|--------------------------------------------------------------|----------|---------------|
| 1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide | 402-40-4 |               |

### New Jersey Right To Know Components

|                                                              | CAS-No.  | Revision Date |
|--------------------------------------------------------------|----------|---------------|
| 1,5-Bis(4-allyldimethylammoniumphenyl)pentan-3-one dibromide | 402-40-4 |               |

### 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.

|                    |                                                        |
|--------------------|--------------------------------------------------------|
| Acute Tox.         | Acute toxicity                                         |
| H300               | Fatal if swallowed.                                    |
| H300 + H310 + H330 | Fatal if swallowed, in contact with skin or if inhaled |
| H310               | Fatal in contact with skin.                            |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 4 |
| Chronic Health Hazard: | * |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 4 |
| Fire Hazard:       | 0 |
| Reactivity Hazard: | 0 |

### Further information

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**Preparation Information**

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

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