

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

Product Description:	<b>S-Butyrylthiocholine iodide</b>
Cat No. :	<b>A12622</b>
Synonyms	(2-Mercaptoethyl)trimethylammonium iodide butyrate
CAS No	1866-16-6
EC No	217-475-7
Molecular Formula	C <sub>9</sub> H <sub>20</sub> I N O S
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

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

Company	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
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E-mail address	begel.sdsdesk@thermofisher.com
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### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

**CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567**

#### Physical hazards

Based on available data, the classification criteria are not met

#### Health hazards

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Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 2 (H315)  
Category 2 (H319)  
Category 3 (H335)

**Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## 2.2. Label elements



Signal Word

Warning

### Hazard Statements

H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H315 - Causes skin irritation

### Precautionary Statements

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

## 2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

## SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Ethanaminium, N,N,N-trimethyl-2-[(1-oxobutyl)thio]-, iodide	1866-16-6	EEC No. 217-475-7	>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

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Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

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<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
<b>Inhalation</b>	Remove to fresh air. Get medical attention. If not breathing, give artificial respiration.
<b>Self-Protection of the First Aider</b>	Use personal protective equipment as required.

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

None reasonably foreseeable.

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

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

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

Thermal decomposition can lead to release of irritating gases and vapors.

#### **Hazardous Combustion Products**

Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Hydrogen iodide.

### **5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

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

Use personal protective equipment as required. Ensure adequate ventilation. Avoid dust formation.

### **6.2. Environmental precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

### **6.3. Methods and material for containment and cleaning up**

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

### **6.4. Reference to other sections**

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Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

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

Keep container tightly closed in a dry and well-ventilated place. Keep refrigerated. Store under an inert atmosphere.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 11  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

#### **Predicted No Effect Concentration (PNEC)**

No information available.

### 8.2. Exposure controls

#### **Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

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## Personal protective equipment

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Nitrile rubber				
Neoprene				
PVC				

**Skin and body protection** Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Particulates filter conforming to EN 143

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Particle filtering: EN149:2001  
When RPE is used a face piece Fit Test should be conducted

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

<b>Physical State</b>	Powder Solid	
<b>Appearance</b>	White	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>Melting Point/Range</b>	172 - 176 °C / 341.6 - 348.8 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flammability (liquid)</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	4-6	50 g/l aq.sol
<b>Viscosity</b>	Not applicable	Solid
<b>Water Solubility</b>	freely soluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid

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Particle characteristics No data available

## 9.2. Other information

Molecular Formula C9 H20 I N O S  
Molecular Weight 317.22  
Evaporation Rate Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Hygroscopic. Light sensitive.

### 10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.  
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid Incompatible products. Excess heat. Avoid dust formation. Exposure to light.

10.5. Incompatible materials Strong oxidizing agents.

10.6. Hazardous decomposition products Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen iodide.

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information No acute toxicity information is available for this product

(a) acute toxicity;  
Oral No data available  
Dermal No data available  
Inhalation No data available

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;  
Respiratory No data available  
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

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<b>(g) reproductive toxicity;</b>	No data available
<b>(h) STOT-single exposure;</b>	Category 3
<b>Results / Target organs</b>	Respiratory system.
<b>(i) STOT-repeated exposure;</b>	No data available
<b>Target Organs</b>	No information available.
<b>(j) aspiration hazard;</b>	Not applicable Solid
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.
<b>Symptoms / effects,both acute and delayed</b>	No information available.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

#### **Ecotoxicity effects**

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

### 12.2. Persistence and degradability

#### **Persistence**

Soluble in water, Persistence is unlikely, based on information available.

### 12.3. Bioaccumulative potential

Bioaccumulation is unlikely

### 12.4. Mobility in soil

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

### 12.6. Endocrine disrupting properties

#### **Endocrine Disruptor Information**

This product does not contain any known or suspected endocrine disruptors

### 12.7. Other adverse effects

#### **Persistent Organic Pollutant**

This product does not contain any known or suspected substance

#### **Ozone Depletion Potential**

This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

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## 13.1. Waste treatment methods

### Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

### Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

### European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

### Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### ADR

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### IATA

Not regulated

#### 14.1. UN number

#### 14.2. UN proper shipping name

#### 14.3. Transport hazard class(es)

#### 14.4. Packing group

### 14.5. Environmental hazards

No hazards identified

### 14.6. Special precautions for user

No special precautions required.

### 14.7. Maritime transport in bulk according to IMO instruments

Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Ethanaminium, N,N,N-trimethyl-2-[(1-oxobutyl)thio]-, iodide	1866-16-6	217-475-7	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification -	DSL	NDSL	AICS	NZIoC	PICCS
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			<b>Active-Inactive</b>					
Ethanaminium, N,N,N-trimethyl-2-[(1-oxobutyl)thio]-, iodide	1866-16-6	X	ACTIVE	X	-	-	X	-

**Legend:** X - Listed '-' - Not Listed

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**Authorisation/Restrictions according to EU REACH**

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Ethanaminium, N,N,N-trimethyl-2-[(1-oxobutyl)thio]-, iodide	1866-16-6	-	-	-

**Seveso III Directive (2012/18/EC)**

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Ethanaminium, N,N,N-trimethyl-2-[(1-oxobutyl)thio]-, iodide	1866-16-6	Not applicable	Not applicable

**Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals**

Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

**National Regulations**

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification**

Water endangering class = 3 (self classification)

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H315 - Causes skin irritation

H319 - Causes serious eye irritation

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H335 - May cause respiratory irritation

## Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

### **Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

### **Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

### **Prepared By**

Health, Safety and Environmental Department

### **Revision Date**

01-Feb-2024

### **Revision Summary**

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

### **Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**