

## SAFETY DATA SHEET

Version 6.4  
Revision Date 09/12/2021  
Print Date 02/11/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3,3'-Diethylthiacyanine iodide

Product Number : 390410  
Brand : Sigma-Aldrich  
CAS-No. : 2197-01-5

**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 ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 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 3), H301  
Acute toxicity, Inhalation (Category 3), H331  
Acute toxicity, Dermal (Category 3), H311  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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

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|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                                                                  |
| H301 + H311 + H331         | Toxic if swallowed, in contact with skin or if inhaled.                                                                          |
| H315                       | Causes skin irritation.                                                                                                          |
| H319                       | Causes serious eye irritation.                                                                                                   |
| H335                       | May cause respiratory irritation.                                                                                                |
| Precautionary statement(s) |                                                                                                                                  |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                            |
| 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/ eye protection/ face protection.                                                    |
| P301 + P310 + P330         | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.                                                             |
| P302 + P352 + P312         | IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.                                          |
| P304 + P340 + P311         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.                         |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.                                                                        |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| P362                       | Take off contaminated clothing and wash 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

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                                  |
|------------------|------------------------------------------------------------------|
| Formula          | : C <sub>19</sub> H <sub>19</sub> IN <sub>2</sub> S <sub>2</sub> |
| Molecular weight | : 466.4 g/mol                                                    |
| CAS-No.          | : 2197-01-5                                                      |
| EC-No.           | : 218-593-1                                                      |

| Component                                                                          | Classification                                                                            | Concentration |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|---------------|
| <b>3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide</b> |                                                                                           |               |
|                                                                                    | Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H301, H331, H311, H315, H319, H335 | <= 100 %      |

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material 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. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### 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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## SECTION 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  
Nitrogen oxides (NO<sub>x</sub>)  
Sulfur oxides  
Hydrogen iodide  
Combustible.

### 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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## SECTION 6: Accidental release measures

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, 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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# **SECTION 7: Handling and storage**

## **7.1 Precautions for safe handling**

### **Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.**Advice on safe handling**

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

### **Advice on protection against fire and explosion**

Provide appropriate exhaust ventilation at places where dust is formed.

### **Hygiene measures**

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

For precautions see section 2.2.

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

### **Storage conditions**

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

### **Storage class**

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

## **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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# **SECTION 8: Exposure controls/personal protection**

## **8.1 Control parameters**

### **Ingredients 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: Dermatrill® (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 EC 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 N99 (US) or type P2 (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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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |                   |
|-------------------|-------------------|
| a) Appearance     | Form: solid       |
| b) Odor           | No data available |
| c) Odor Threshold | No data available |
| d) pH             | No data available |

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|                                                 |                                                 |
|-------------------------------------------------|-------------------------------------------------|
| e) Melting point/freezing point                 | Melting point/range: > 300 °C (> 572 °F) - lit. |
| 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) Density                                      | No data available                               |
| Relative density                                | No data available                               |
| n) Water solubility                             | No data available                               |
| o) Partition coefficient: n-octanol/water       | No data available                               |
| p) Autoignition 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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## SECTION 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

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

LC50 Inhalation - 4 h - 0.51 mg/l

(Acute toxicity estimate)

LD50 Dermal - 300 mg/kg

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

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

NTP: No ingredient 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 on OSHA's list of regulated carcinogens.

#### Reproductive toxicity

No data available

No data available

#### Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

### 11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 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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## SECTION 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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## SECTION 14: Transport information

### DOT (US)

UN number: 2811 Class: 6.1

Packing group: III

Proper shipping name: Toxic solids, organic, n.o.s. (3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

### IMDG

UN number: 2811 Class: 6.1

Packing group: III

EMS-No: F-A, S-A

Proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide)

### IATA

UN number: 2811 Class: 6.1

Packing group: III

Proper shipping name: Toxic solid, organic, n.o.s. (3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide)

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## SECTION 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

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No SARA Hazards

#### Massachusetts Right To Know Components

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

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

#### Pennsylvania Right To Know Components

3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide

CAS-No.  
2197-01-5

Revision Date

3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide

CAS-No.  
2197-01-5

Revision Date

#### New Jersey Right To Know Components

3-Ethyl-2-[(3-ethyl-3H-benzothiazol-2-ylidene)methyl]benzothiazolium iodide

CAS-No.  
2197-01-5

Revision Date

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## SECTION 16: Other information

### 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.

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