

SAFETY DATA SHEET

Version 6.8 Revision Date 09/08/2024 Print Date 09/09/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

	Product name	:	3,3'-Diethylthiatricarbocyanine iodide
	Product Number Brand CAS-No.	-	381306 Aldrich 3071-70-3
1.2	2 Relevant identified uses of the substance or mixture and uses advised against		
	Identified uses	:	Laboratory chemicals, Synthesis of substances
	Uses advised against	:	The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 Fax	-	+1 314 771-5765 +1 800 325-5052
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 4), H302 Acute toxicity, Inhalation (Category 4), H332 Acute toxicity, Dermal (Category 4), H312 Skin irritation (Category 2), H315

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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	Warning
Hazard Statements H302 + H312 + H332 H315 H319 H335	Harmful if swallowed, in contact with skin or if inhaled. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.
Precautionary Statements P261 P264 P270 P271 P280	Avoid breathing dust. Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product. Use only outdoors or in a well-ventilated area. Wear protective gloves/ protective clothing/ eye protection/ face
P301 + P312 + P330	protection. IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water.Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
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 P337 + P313 P362	If skin irritation occurs: Get medical advice/ attention. If eye irritation persists: Get medical advice/ attention. Take off contaminated clothing and wash before reuse.
P403 + P233 P405 P501	Store in a well-ventilated place. Keep container tightly closed. Store locked up. 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 Synonyms

: DTTCI DiSC2(7) DTTC iodide 3-Ethyl-2-[7-(3-ethyl-2-benzothiazolinylidene)-1,3,5heptatrienyl]benzothiazolium iodide

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Formula	: $C_{25}H_{25}IN_2S_2$	
Molecular weight	: 544.51 g/mol	
CAS-No.	: 3071-70-3	
EC-No.	: 221-342-9	

Component	Classification	Concentration	
3-Ethyl-2-[7-(3-ethyl-3H-benzothiazol-2-ylidene)hepta-1,3,5- trienyl]benzothiazolium iodide			
	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H302, H332, H312, H315, H319, H335	<= 100 %	

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given. Aldrich - 381306

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5.2 Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx) Sulfur oxides Hydrogen iodide Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions Tightly closed. Dry.

rightly closed. Dry

Light sensitive.

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Storage class

Storage class (TRGS 510): 11: Combustible Solids

7.3 Specific end use(s)

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

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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). Safety glasses

Skin protection

Handle with impervious gloves.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested:KCL 741 Dermatril® L

Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested:KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type P2 The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented. required when dusts are generated.

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Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

	· · · · · · · · · · ·	
a)	Appearance	Form: powder
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	рН	No data available
e)	Melting point/freezing point	Melting point/ range: 211 °C (412 °F) - dec.
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
I)	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

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SECTION 10: Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

- 10.3 Possibility of hazardous reactions No data available
- **10.4 Conditions to avoid** no information available
- **10.5 Incompatible materials** Strong oxidizing agents
- **10.6 Hazardous decomposition products** In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available LC50 Inhalation - 4 h - 1.5 mg/l - dust/mist

(Acute toxicity estimate) LD50 Dermal - 1,100 mg/kg No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation Remarks: 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.

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- 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

RTECS: DL7045000

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

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 Endocrine disrupting properties No data available

12.7 Other adverse effects

No data available

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SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

ΙΑΤΑ

Not dangerous goods

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards	:	Acute Health Hazard
SARA 313	:	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.

US State Regulations

Massachusetts Right To Know

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

Maine Chemicals of High Concern

Product does not contain any listed chemicals

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Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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