

Safety Data Sheet

#34904481 · Full 16-section SDS

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

PRODUCT	CAS NUMBER	FORMULA	VERSION	REVISION DATE
Butyrylthiocholine iodide	1866-16-6	(CH ₃) ₃ N(I)CH ₂ CH ₂ SC(=O)CH ₂ CH ₂ CH ₃	10	01 Sep 2026

SECTION 1

Identification

1.1 Product identifier

Product name Butyrylthiocholine iodide

CAS number 1866-16-6

EC / EINECS number *Not applicable*

Chemical formula (CH₃)₃N(I)CH₂CH₂SC(=O)CH₂CH₂CH₃

Molecular weight 317.23

SMILES CCCC(=O)SCC[N+](C)(C)C.[I-]

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

For research and development. Laboratory chemicals. Manufacture of substances. Not suitable for human or veterinary purposes.

1.3 Details of the supplier of the safety data sheet

Molekula Limited
1 Millennium Way, Newton Aycliffe
Durham, DL5 6JW, United Kingdom
info@molekula.com · +44 (0) 3302 000333

1.4 Emergency telephone number

0344 892 0111 — National Poisons Information Service (NPIS) (United Kingdom — for healthcare professionals (via TOXBASE))

SECTION 2

Hazard identification

2.1 Classification of the substance or mixture

Skin Irrit. 2; H315

Eye Irrit. 2; H319

STOT SE 3; H335

2.2 Label elements



WARNING

CODE	HAZARD STATEMENT
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H315	Causes skin irritation
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H319	Causes serious eye irritation
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H335	May cause respiratory irritation
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CODE	PRECAUTIONARY STATEMENT
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P261	Avoid breathing dust/fume/gas/mist/vapours/spray
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P280	Wear protective gloves/protective clothing/eye protection/face protection
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P302+352	IF ON SKIN: Wash with soap and water
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P304+341	IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing
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P305+351+338	IF IN EYES: Rinse with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing
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P308+313	IF exposed or concerned: Get medical advice/attention
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2.3 Other hazards

Not applicable

SECTION 3

Composition / information on ingredients

3.1 Substances

Name	Butyrylthiocholine iodide
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CAS number	1866-16-6
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EC number	217-475-7
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Concentration / purity	~100%
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Classification according to Regulation (EC) No 1272/2008	Skin Irrit. 2; H315 Eye Irrit. 2; H319 STOT SE 3; H335
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Hazard statements	H315, H319, H335
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Acute toxicity estimate (ATE)	<i>No data available</i>
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Impurities / stabilising additives	<i>Not applicable</i>
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SECTION 4

First-aid measures

4.1 Description of first aid measures

Inhalation	Fresh air
Skin contact	Remove contaminated clothing; rinse skin with water/shower
Eye contact	Rinse with plenty of water; remove contact lenses
Ingestion	After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel. First aiders/ medical personnel need to protect themselves.

4.2 Most important symptoms and effects, both acute and delayed

Treat symptomatically

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	Water, foam, CO ₂ , dry powder
Unsuitable extinguishing media	No specific firefighting procedure given

5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides, sulfur oxides, hydrogen iodide; combustible; hazardous combustion gases possible

5.3 Advice for firefighters

Use self-contained breathing apparatus; suppress gases/vapors with water spray; prevent groundwater contamination

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Avoid inhalation of dust; evacuate danger area; consult expert

6.2 Environmental precautions

Do not let product enter drains

6.3 Methods and material for containment and cleaning up

Cover drains; collect spills; dispose properly; avoid dust generation

6.4 Reference to other sections

For specific precautions, see Section 8 and Section 13.

SECTION 7

Handling & storage

7.1 Precautions for safe handling

Not applicable

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature -15 to -20 °C

Conditions for safe storage (incompatibilities) Tightly closed, dry, air/moisture/light sensitive; store under inert gas; hygroscopic

7.3 Specific end use(s)

See Section 1.2.

SECTION 8

Exposure controls / personal protection

8.1 Control parameters

Occupational exposure limits (OEL / WEL) Not applicable

DNEC/PNEC data Not applicable

8.2 Exposure controls

Eye / face protection Safety glasses
Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.

Skin / hand protection Gloves: Nitrile Rubber, 0.11mm (480 mins).

Respiratory protection Dust mask (FFP2/FFP3)
Keep self-contained breathing apparatus readily available for emergency use. Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided. Respiratory equipment: Reusable Air-Purifying Respirator (APR). Filter type: ABEK. Standard: EN 14387.

Other protection No data available

Environmental exposure controls No data available

SECTION 9

Physical & chemical properties

9.1 Information on basic physical and chemical properties

Appearance / physical state Not applicable

Colour Not applicable

Odour	<i>Not applicable</i>
Melting / freezing point	<i>Not applicable</i>
Boiling point	<i>Not applicable</i>
Flammability	<i>No data available</i>
Lower and upper explosion limit	<i>No data available</i>
Flash point	<i>Not applicable</i>
Auto-ignition temperature	<i>Not applicable</i>
Decomposition temperature	<i>No data available</i>
pH	<i>Not applicable</i>
Acidity	Neutral DERIVED FROM: LITERATURE
Kinematic viscosity	<i>No data available</i>
Solubility	<i>Not applicable</i>
Partition coefficient n-octanol/water (log value)	<i>Not applicable</i>
Vapour pressure	<i>Not applicable</i>
Density (g/mL)	1 g/mL DERIVED FROM: LITERATURE
Relative vapour density	<i>No data available</i>
Particle characteristics	<i>No data available</i>

9.2 Other information

No data available

SECTION 10

Stability & reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

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.

10.3 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

See section 5

SECTION 11

Toxicological information

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

Acute toxicity (LD50 / LC50) *No data available*

Skin corrosion / irritation *No data available*

Eye corrosion / irritation *No data available*

Respiratory / skin sensitisation *No data available*

Carcinogenicity *No data available*

Mutagenicity *No data available*

Reproductive toxicity *No data available*

STOT (single / repeated exposure) *No data available*

Aspiration hazard *No data available*

11.2 Information on other hazards

This product does not contain any known or suspected endocrine disruptors.

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

Not applicable

12.6 Endocrine disrupting properties

See Section 11.2.

12.7 Other adverse effects

No data available

SECTION 13

Disposal considerations

13.1 Waste treatment methods

Dispose of in accordance with local/national regulations

SECTION 14

Transport information

14.1 UN number or ID number

Not applicable

14.2 UN proper shipping name

Not applicable

14.3 Transport hazard class(es)

Not applicable

14.4 Packing group

Not applicable

14.5 Environmental hazards

Not applicable

14.6 Special precautions for user

Special precautions for user *Not applicable*

Transport category *Not applicable*

Tunnel code *Not applicable*

Packing instruction (ADR) *Not applicable*

Packing instruction (IMDG) *Not applicable*

14.7 Maritime transport in bulk according to IMO instruments

No data available

SECTION 15

Regulatory information

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

Substance-specific regulations (e.g. licences) *No data available*

REACH code Y110

ECHA notification *Not applicable*

15.2 Chemical safety assessment

Not required

SECTION 16

Other information

Revision notes / other information

This SDS replaces version Version 1 Date of issue: 3/29/2019

This Safety Data Sheet was generated automatically from the data Molekula holds against this product, in the 16-section GHS/CLP format. Fields shown as "No data available" carry no recorded value; fields shown as "Not applicable" were assessed as not relevant to this substance. For queries, contact Molekula at info@molekula.com.