

Safety Data Sheet

#12059739 · 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
2,5-Bis-(5'-tert-butylbenzoxazolyl)-2'-thiophene	7128-64-5	C26H26N2O2S	10	09 Aug 2026

SECTION 1

Identification

1.1 Product identifier

Product name 2,5-Bis-(5'-tert-butylbenzoxazolyl)-2'-thiophene

CAS number 7128-64-5

EC / EINECS number 230-426-4

Chemical formula C26H26N2O2S

Molecular weight 430.56

SMILES N1=C(OC2=CC=C(C=C12)C(C)(C)C)C=3SC(=CC3)C4=NC5=CC(=CC=C5O4)C(C)(C)C

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

Acute Tox. 4; H332

2.2 Label elements



WARNING

CODE	HAZARD STATEMENT
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H332	Harmful if inhaled
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CODE	PRECAUTIONARY STATEMENT
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P261	Avoid breathing dust/fume/gas/mist/vapours/spray
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P271	Use only outdoors or in a well-ventilated area
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P280	Wear protective gloves/protective clothing/eye protection/face protection
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P308+P313	IF exposed or concerned: Get medical advice/attention
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2.3 Other hazards

Not a PBT or vPvB substance under REACH Annex XIII.

Does not contain components considered to have endocrine-disrupting properties

SECTION 3

Composition / information on ingredients

3.1 Substances

Name	2,5-Bis-(5'-tert-butylbenzoxazolyl)-2'-thiophene
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CAS number	7128-64-5
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EC number	230-426-4
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Concentration / purity	~100%
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Classification according to Regulation (EC) No 1272/2008	Acute Tox. 4; H332
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Hazard statements	H332
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Acute toxicity estimate (ATE)	No data available
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Impurities / stabilising additives	Not specified
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SECTION 4

First-aid measures

4.1 Description of first aid measures

Inhalation	Remove to fresh air, rest comfortably; give oxygen/artificial respiration if needed; seek medical advice if breathing difficulties persist
Skin contact	Remove contaminated clothing (unless stuck), wash immediately with plenty of water; consult doctor if irritation persists
Eye contact	Rinse immediately with water, remove contact lenses if easy, continue rinsing; seek medical advice if irritation persists
Ingestion	Rinse mouth with water; do not induce vomiting; seek medical advice

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

Dust may cause respiratory irritation (inhalation), skin irritation (dust in folds/tight clothing), eye irritation (redness, itching, tears), and digestive tract irritation (abdominal pain, nausea)

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	Foam, dry powder, carbon dioxide, water spray, sand
Unsuitable extinguishing media	Heavy water stream

5.2 Special hazards arising from the substance or mixture

Combustible.

Carbon Monoxide (CO)

Carbon Dioxide (CO₂)

Nitrogen oxides (NO_x)

Sulphur oxide (SO_x).

Development of hazardous combustion gases or vapours is possible in the event of fire.

5.3 Advice for firefighters

Keep container closed, away from heat/sparks; use water spray for cooling; avoid environmental water contamination; do not enter fire area without protective equipment

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Isolate from fire, avoid dust, eliminate ignition sources; evacuate unnecessary personnel; mark contaminated area; wear PPE (respiratory, protective clothing)

6.2 Environmental precautions

Prevent entry into sewers/public waters; notify authorities if contamination occurs

6.3 Methods and material for containment and cleaning up

Sweep/shovel into containers; ventilate area thoroughly; avoid dust spread

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

For precautions see section 2.2.

Do not handle until all safety precautions have been read and understood.

Do not handle broken packages without protective equipment.

Keep containers tightly closed. Immediate first aid is necessary. Wear protective clothing, gloves, eye and face protection.

Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Do not reuse empty containers.

General hygiene - Observe good chemical hygiene practices. Remove contaminated clothing immediately and wash

skin with soap and water. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature	Ambient
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Conditions for safe storage (incompatibilities)	Original container, cool, well-ventilated, away from heat/sunlight; keep closed; incompatible with strong oxidizers/acids/ignition sources
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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 specified

DNEC/PNEC data

DNEL:
Chronic effects systemic (Dermal): DNEL = 7.1mg/kg bw/day
Chronic effects systemic (Inhalation) DNEL = 3mg/m

PNEC:
Fresh water: PNEC = 0.2mg/L
Microorganisms in sewage treatment: PNEC = 1mg/L
Soil (Agriculture): PNEC = 629000mg/kg soil dw
Marine water: PNEC = 0.02mg/L
Marine water (Sediment): PNEC = 316000mg/kg sediment dw

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 Long-sleeved protective clothing (EN ISO 13982); disposable nitrile gloves (0.11 mm, >480 min permeation, EN 374)

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 Powder
DERIVED FROM: LITERATURE

Colour Yellow
DERIVED FROM: LITERATURE

Odour Not known
DERIVED FROM: LITERATURE

Melting / freezing point 199 - 201 °C
DERIVED FROM: LITERATURE

Boiling point *No data available*

Flammability *No data available*

Lower and upper explosion limit	<i>No data available</i>
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Flash point	<i>Not applicable</i>
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Auto-ignition temperature	Not specified DERIVED FROM: LITERATURE
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Decomposition temperature	<i>No data available</i>
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pH	<i>No data available</i>
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Acidity	Neutral DERIVED FROM: LITERATURE
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Kinematic viscosity	<i>No data available</i>
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Solubility	1 g/l at 20 °C DERIVED FROM: LITERATURE
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Partition coefficient n-octanol/water (log value)	log Pow: > 6.5 at 23 °C - Potential bioaccumulation DERIVED FROM: LITERATURE
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Vapour pressure	<i>No data available</i>
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Density (g/mL)	1.272 g/mL DERIVED FROM: LITERATURE
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Relative vapour density	<i>No data available</i>
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Particle characteristics	<i>No data available</i>
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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

Heat, sparks, flames, direct sunlight, strong oxidizers, strong acids

10.5 Incompatible materials

Strong oxidizers, strong acids, ignition sources

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)	LD50 Oral - Rat - > 10,000 mg/kg
	LC50 Inhalation - Rat - male and female - 4 h - > 1.8 mg/l - dust/mist
	Dermal: No data available
Skin corrosion / irritation	Skin - Rabbit Result: No skin irritation - 24 h
Eye corrosion / irritation	Eyes - Rabbit Result: No eye irritation
Respiratory / skin sensitisation	Maurer optimisation test - Guinea pig Result: Not a skin sensitiser.
Carcinogenicity	Test Type: gene mutation test Test system: Chinese hamster fibroblasts Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476 Result: negative
	Test Type: Ames test Test system: S. typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471 Result: negative
Mutagenicity	<i>Not applicable</i>
Reproductive toxicity	<i>Not applicable</i>
STOT (single / repeated exposure)	<i>No data available</i>
Aspiration hazard	<i>No data available</i>

11.2 Information on other hazards

The substance does not contain components considered to have endocrine-disrupting properties.

SECTION 12

Ecological information

12.1 Toxicity

Toxicity to Fish

LC50 - Danio rerio (zebra fish) - > 100 mg/l - 96 h (Lit.)

Toxicity to Algae

EC50 - Pseudokirchneriella subcapitata - > 100 mg/l - 72 h (Lit.)

Toxicity to Bacteria

Remarks: (ECHA) (2,5-Thiophenediylbis(5-tert-butyl-1,3-benzoxazole))

Chronical Toxicity

NOEC - Daphnia magna (Water flea) - > 10 mg/l - 22 d (Lit.)

12.2 Persistence and degradability

Aerobic: Exposure time 28 d Result: 4 % =Not readily biodegradable.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

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

Sweep/shovel into containers for disposal (see Section 6.3).
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 applicable

SECTION 16

Other information

Revision notes / other information *Not applicable*

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.