SAFETY DATA SHEET (SDS)

in accordance with Regulation (EC) No 1907/2006 (REACH), Annex II — Regulation (EU) 2020/878

Date: 02.11.2026 | Version: 7 | EN

benzothiazole-2-thiol

3H-1,3-benzothiazole-2-thione

CAS 149-30-4

$C_7H_5NS_2$ | EC 205-736-8

MOLAR MASS	LOGP
167.30	2.4

HAZARD CLASSIFICATION (GHS / CLP)



Warning

H317 | H400 | H410

Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.

1. Identification of the substance/mixture and of the company/undertaking

1.1 Substance name	benzothiazole-2-thiol
1.1 IUPAC name	3H-1,3-benzothiazole-2-thione
1.1 CAS number	149-30-4
1.1 EC number	205-736-8
1.1 PubChem CID	697993
1.1 InChIKey	YXIWHUQXZSMYRE-UHFFFAOYSA-N
1.1 SMILES	C1=CC=C2C(=C1)NC(=S)S2
1.1 Molecular formula	$C_7H_5NS_2$ [7]
1.1 Molar mass	167.3 g/mol [7]
1.1 Exact mass	166.9863 Da [7]

1.2 Uses

For laboratory and research purposes. Not for use in the production of food, medicines or cosmetics without appropriate authorisation.

1.3 Details of the supplier

REFERENCE COPY — NO SUPPLIER DETAILS — NOT FOR DISTRIBUTION	Supplier details are not included in this reference copy. The supplier placing the substance on the market must complete this section and remains responsible for the sheet under REACH. MolGod.org prepares documentation and is not the supplier of this substance.

1.4 Emergency telephone number

Emergency telephone	112 (EU-wide emergency number)

Contact the poison centre designated in the country of placing on the market (CLP Art. 45).

2. Hazards identification

GHS:



PPE:



Warning

Hazard statements (H) [3][4][10]

H317	May cause an allergic skin reaction
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

Precautionary statements (P) [3][4][10]

P261	Avoid breathing dust/fume/gas/mist/vapours/spray
P272	Contaminated work clothing should not be allowed out of the workplace
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P302+P352	IF ON SKIN: Wash with plenty of water
P321	Specific treatment
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P362+P364	Take off contaminated clothing
P391	Collect spillage
P501	Dispose of contents/container to an approved waste collection point

Hazard class scope limited to the harmonised classification (CLP Annex VI); classes outside the harmonised entry may require supplier self-classification (CLP Art. 4(3)) — verify with the supplier safety data sheet.

WORKING DRAFT 工作草稿

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	149-30-4
EC number	205-736-8
Molecular formula	$C_7H_5NS_2$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	613-108-00-3

4. First aid measures



Inhalation

Move the affected person to fresh air. Keep at rest. If not breathing: artificial respiration (qualified personnel only). [1][2][13]

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). [1][2][13]

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [1][2][13]

Ingestion

Do NOT induce vomiting (unless directed by a physician). Rinse mouth with water. Never give anything by mouth to an unconscious person. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][13]

Symptoms and effects

No specific symptoms described in the literature. [3][10]

Notes for physician

Requires verification

Emergency numbers: Emergency: 112 (EU-wide). Poison centre: as designated in the country of placing on the market (CLP Art. 45).

5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO2, dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO2, NOx, SOx. [14]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	200°C [7]
Auto-ignition temperature	628°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust. [1][2][13]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][13]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [1][2][13]
Related sections	8; 13

WORKING DRAFT 工作草案

7. Handling and storage

Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2][13]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2][13]
Humidity	Store in a dry place (<60% RH). [1][2][13]
Light	Protect from direct sunlight. [1][2][13]
Incompatible materials	Strong oxidizers. [14]

8. Exposure controls/personal protection

8.1 Control parameters

OEL — NDS (Poland)	No NDS (OEL) value in the available working list — verify in the current MRPiPS regulation before use; do not assume the absence of a limit value.
OEL (EU)	The EU OEL value has not been verified against the available dataset — check the IOELV/BOELV directives; do not assume the absence of a value.
DNEL	No data available.
PNEC	No data available.

8.2 Personal protective equipment (PPE) [5][6][15]



Chemical-resistant protective gloves
EN ISO 374-1:2016+A1:2018
nitrile (min. 0.11 mm)



Closed safety spectacles or goggles
EN ISO 16321-1:2022 / EN 166:2001



Closed safety footwear with toe protection
EN ISO 20345:2022 (S2/S3)

9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Solid	
Colour	Pale, yellow monoclinic needles or leaflets [7]	
Odour	Disagreeable odor [7]	
pH (1% aqueous solution)	No data available.	
Melting point	181.1423°C [8] [7]	
Boiling point	No data available.	
Flash point	200°C (experimental data) [7]	
Flammability	No data available.	
Lower and upper explosion limit	Not applicable (REACH 9.1(g))	
Density (20°C)	1.42 g/cm³ [7]	
Vapour pressure	0 kPa (0.000464 mmHg) (experimental data) [7]	
Relative vapour density	Not applicable (REACH 9.1(q))	

WORKING DRAFT 工作草稿

Property (item 9.1)	Value	Source
Kinematic viscosity	Not applicable (REACH 9.1(l))	
Auto-ignition temperature	628°C (experimental data) [7]	
Decomposition temperature	Not applicable	
Water solubility	0.12 g/L, 24°C [7]	
Particle characteristics	The particle size distribution has not been determined for this commercial form — required under Annex II 9.1(r); to be completed from the supplier's specification.	
Partition coefficient n-octanol/water (log value)	2.4 [9]	
Molar mass	167.3 g/mol [7]	
Molecular formula	$C_7H_5NS_2$ [7]	
Lipinski rule (RO5)	PASS	

Where a property above reads "No data available", no measured value was found in the public sources consulted for this substance. The property has not been determined by MolGod.org and no value is inferred. "Not applicable" means the property has no meaning for this substance in the form supplied.

10. Stability and reactivity

Reactivity	Stable under normal storage and handling conditions.
Chemical stability	Thermally stable under recommended conditions.
Hazardous reactions	No hazardous reactions known under normal conditions.
Conditions to avoid	High temperatures, direct sunlight, moisture.
Incompatible materials	Strong oxidizers.
Decomposition products	Thermal decomposition products: CO, CO2, NOx, SOx.

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Eye irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Sensitisation	Skin, Category 1 (H317): May cause an allergic skin reaction. [3][10]
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
Carcinogenicity	No harmonised CLP classification as carcinogenic; for carcinogenicity assessment see the IARC classification below. [18]
IARC classification (carcinogenicity)	IARC Group 2A — probably carcinogenic to humans. [local snapshot — not verified against the current IARC list] [18]
Reproductive toxicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
STOT — single exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]
STOT — repeated exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]

WORKING DRAFT 工作草案

Aspiration hazard	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) [3][10]

12. Ecological information

Aquatic toxicity	Harmonised classification (CLP Annex VI): H400 — Very toxic to aquatic life (Aquatic Acute 1); H410 — Very toxic to aquatic life with long lasting effects (Aquatic Chronic 1) (M-factor for acute/chronic cat. 1 — to be verified per Table 3 of Annex VI, if assigned.). LC_{50} (fish): 0.42 mg/L (Oncorhynchus mykiss, 96 h). EC_{50} (Daphnia): 2.9 mg/L (Daphnia magna, 48 h). EC_{50} (algae): 0.23 mg/L (Raphidocelis subcapitata, 96 h) [19]
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 2.4 [9]. Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). [16][17]
Mobility in soil	No data available.
PBT/vPvB assessment	Insufficient data to assess PBT/vPvB.
Endocrine disrupting properties	No information.

13. Disposal considerations

Disposal method	Hand over for disposal to licensed contractors in accordance with national and local regulations. Do not discharge into sewers.
Waste code (EWC)	16 05 06* — Laboratory and analytical chemicals (e.g. chemical reagents) containing hazardous substances. Verification of the EWC code required. [12]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information

UN number	VERIFICATION REQUIRED — no verified UN assignment.
Environmental hazard	CLP classification (H400/H410) indicates aquatic environmental hazard — marine pollutant marking may be required; confirm per ADR 2.2.9 / IMDG criteria [3]
Special precautions	Handle as dangerous goods according to the assigned class (ADR/IMDG/IATA); apply the precautions appropriate to that class.
CN/HS code	CN/HS code: verification required in the Eurostat Combined Nomenclature.
Notes	Transport classification not verified. Do not assume the absence of restrictions — check ADR/IMDG/IATA before shipping.
Environmentally hazardous (mark: fish and tree)	Yes

15. Regulatory information

SVHC status	SVHC status not verified against the available dataset — check the current ECHA Candidate List; do not assume absence. [1]
REACH Annex XIV	Not verified against the ECHA Authorisation List — check REACH Annex XIV. [1]
REACH Annex XVII	Not confirmed in the available Annex XVII dataset — verify against the current ECHA list before placing on the market; do not assume absence of restriction. [1]
IARC classification (carcinogenicity)	IARC Group 2A — probably carcinogenic to humans.

WORKING DRAFT · 工作草稿

16. Other information

Legal status of classification: harmonised under CLP Annex VI — Reg. (EC) No 1272/2008 (as at the date of issue).Entries with an entry-into-force date after 02.11.2026 were omitted as future (not yet applicable).

Data aggregated automatically from public reference databases (PubChem, ECHA, NIST and others).

Scientific citations (1)

NTP Toxicology and Carcinogenesis Studies of 2-Mercaptobenzothiazole (CAS No. 149-30-4) in F344/N Rats and B6C3F1 Mice (Gavage Studies).. (1988).

Full text of H statements

H317	May cause an allergic skin reaction
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

Full text of P statements

P261	Avoid breathing dust/fume/gas/mist/vapours/spray
P272	Contaminated work clothing should not be allowed out of the workplace
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P302+P352	IF ON SKIN: Wash with plenty of water
P321	Specific treatment
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P362+P364	Take off contaminated clothing
P391	Collect spillage
P501	Dispose of contents/container to an approved waste collection point

Abbreviations

ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service
CLP	Classification, Labelling and Packaging (Reg. (EC) 1272/2008)
CMR	Carcinogenic, Mutagenic, toxic to Reproduction
DNEL	Derived No-Effect Level
EC	European Community number
EPI	Personal protective equipment
GHS	Globally Harmonized System
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods Code
SDS	Safety Data Sheet
LC50	Lethal Concentration, 50%
LD50	Lethal Dose, 50%
NDS	Maximum admissible concentration (workplace, PL)
NDSCh	Short-term exposure limit (PL)
OEL	Occupational Exposure Limit
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (Reg. (EC) 1907/2006)

WORKING DRAFT 工作草稿

STOT	Specific Target Organ Toxicity
SVHC	Substance of Very High Concern
TPSA	Topological Polar Surface Area
vPvB	very Persistent and very Bioaccumulative

Version history

v7 (02.11.2026)	Based on ECHA harmonised classification (Annex VI to CLP, ATP 23).

References

[1] EP and Council. Reg.(EC) No 1907/2006 (REACH). Art.31, Annex II. OJ EU L 396/2006. URL: https://eur-lex.europa.eu/eli/reg/2006/1907/oj Accessed: 2026-11-02.

[2] European Commission. Reg.(EU) 2020/878 — amending Annex II REACH. OJ EU L 203/2020. From 01.01.2023. URL: https://eur-lex.europa.eu/eli/reg/2020/878/oj Accessed: 2026-11-02.

[3] EP and Council. Reg.(EC) 1272/2008 (CLP) + ATP 23. OJ EU L 353/2008. (2026-07-07) URL: https://eur-lex.europa.eu/eli/reg/2008/1272/oj Accessed: 2026-11-02.

[4] United Nations. GHS Rev.9. ST/SG/AC.10/30/Rev.9. New York and Geneva: United Nations, 2021. URL: https://unece.org/transport/dangerous-goods/ghs-rev9-2021 Accessed: 2026-11-02.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-11-02.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-11-02.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/697993

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=149-30-4

[9] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: https://hbcp.chemnetbase.com

[10] ECHA. European Chemicals Agency — harmonised classification inventory (CLP Annex VI). URL: https://echa.europa.eu

[11] ECHA. REACH Registration Dossier (registered substance, acute toxicity study record). Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/registration-dossier

[12] European Commission. Decision 2000/532/EC establishing a list of wastes (European Waste Catalogue). OJ EU L 226/3. URL: https://eur-lex.europa.eu/eli/dec/2000/532/oj

[13] European Chemicals Agency (ECHA). Guidance on the Compilation of Safety Data Sheets. Version 4.0. Helsinki: European Chemicals Agency, 2020. URL: https://echa.europa.eu/documents/10162/2324906/sds_en.pdf

[14] Urben, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.

[15] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.

[16] ECHA. Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB Assessment. Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

[17] European Parliament and Council. Regulation (EC) No 1907/2006 (REACH), Annex XIII — Criteria for the identification of PBT and vPvB substances. OJ EU L 396/2006 (consolidated). URL: https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20140410

[18] IARC. IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. Lyon: International Agency for Research on Cancer. URL: https://monographs.iarc.who.int

[19] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: https://cfpub.epa.gov/ecotox/

[20] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-11-02.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=149-30-4

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL111654

NFPA 704 (supplementary information — NFPA/USA system; not a required element of an EU safety data sheet under REACH Annex II)



Legal notice: This document was generated automatically from data provided by PubChem (NIH), ECHA, NIST WebBook, ChemSpider (RSC) and other public databases. It DOES NOT REPLACE an approved Safety Data Sheet (SDS) compliant with Regulation (EC) No 1907/2006 (REACH). Before using the substance, verify the data against the manufacturer's current SDS.

Generator: Document generated automatically from ECHA harmonised classification (Annex VI to CLP) and public physicochemical databases.
Author: www.MolGod.org — platform for automated safety data sheets (SDS).
Issue date: 02.11.2026 | Document version: 7

WORKING