

SAFETY DATA SHEET (SDS)

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

Date: 15.07.2026 | Version: 2 | EN

5-[(3aS,4S,6aR)-2-oxo-1,3,3a,4,6,6a-hexahydrothieno[3,4-d]imidazol-4-yl]pentanoic acid

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CAS 58-85-5

$C_{10}H_{16}N_2O_3S$

MOLAR MASS

244.31

LOGP

0.30
(XLogP3,
PubChem)

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

1.1 Substance name

—

1.1 IUPAC name

5-[(3aS,4S,6aR)-2-oxo-1,3,3a,4,6,6a-hexahydrothieno[3,4-d]imidazol-4-yl]pentanoic acid

1.1 CAS number

58-85-5

1.1 EC number

No data

1.1 PubChem CID

171548

1.1 InChIKey

YBJHBAHKTGYVGT-ZKWXMUAHSA-N

1.1 SMILES

C1[C@H]2[C@@H]([C@@H](S1)CCCC(=O)O)NC(=O)N2

1.1 Molecular formula

$C_{10}H_{16}N_2O_3S$

1.1 Molar mass

244.31 g/mol

1.1 Exact mass

—

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

Supplier details have not been configured (MOL-GOD → Label generator → Producer details).

1.4 Emergency telephone number

Emergency telephone

+48 42 657 99 00

Toxicological Information Centre (CIT), Łódź — available 24/7

2. Hazards identification

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	58-85-5
Molecular formula	$C_{10}H_{16}N_2O_3S$
Concentration	$\geq 99\%$

4. First aid measures



Inhalation

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

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes).

Eye contact

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

Ingestion

Do NOT induce vomiting (unless directed by a physician). Rinse mouth with water. Never give anything by mouth to an unconscious person. Poison Centre Łódź: +48 42 657 99 00 (24/7). Emergency number: 112.

Symptoms and effects

No specific symptoms described in the literature.

Notes for physician

Symptomatic treatment. No specific antidote.

Emergency numbers: CIT Łódź: +48 42 657 99 00 (24/7) | Emergency: 112

5. Firefighting measures

Suitable extinguishing media	Adapt extinguishing media to surroundings. CO ₂ , dry powder, foam.
Unsuitable extinguishing media	No specific restrictions.
Specific hazards	Thermal decomposition products: CO, CO ₂ , NO _x , SO _x .
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.

6. Accidental release measures

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

7. Handling and storage

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

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)



9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Solid	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	232°C	
Boiling point	No data available.	
Flash point	No data available.	
Density (20°C)	No data available.	
Vapour pressure (20°C)	No data available.	
Water solubility (20°C)	No data available.	
log Kow (XLogP3)	0.3	
TPSA	104 Å ²	PubChem (NIH)
HBD / HBA	No data available. / No data available.	
Rotatable bonds	No data available.	
Molar mass	244.31 g/mol	PubChem (NIH)
Molecular formula	C ₁₀ H ₁₆ N ₂ O ₃ S	PubChem (NIH)

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, strong bases, Base metals (hydrogen evolution).
Decomposition products	Thermal decomposition products:CO, CO ₂ , NO _x , SO _x .

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	No data available.
Eye irritation	No data available.
Sensitisation	No data available.
Mutagenicity	No data available.
Carcinogenicity	No data available.
IARC classification (carcinogenicity)	No individual IARC monograph for this CAS — this is not confirmation of the absence of carcinogenicity (cf. CLP/GHS classification in section 2).
Reproductive toxicity	No data available.
STOT — single exposure	No data available.
STOT — repeated exposure	No data available.
Aspiration hazard	No data available.

12. Ecological information

Aquatic toxicity	No data available.
Persistence / biodegradability	No data available.
Bioaccumulative potential	LogP = 0.3. Low bioaccumulation potential.
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.
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	No environmental hazard indicated by GHS classification. Verification required.
Special precautions	Verification required.
CN/HS code	CN/HS code: verification required in the Eurostat Combined Nomenclature.

15. Regulatory information

SVHC status	SVHC status not verified against the full ECHA Candidate List (verification required) — check the ECHA Candidate List
REACH Annex XIV	Not verified against the ECHA Authorisation List — check REACH Annex XIV.
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.
Verification date	2026-07-15

16. Other information

Legal status of the harmonised classification: CLP — Regulation (EC) No 1272/2008, Annex VI (current ECHA harmonised inventory, as at the issue date of this sheet). Entries entering into force after 15.07.2026 were omitted as future (not yet applicable).

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

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

Version history

v2 (15.07.2026)	Prepared on the basis of the ECHA harmonised classification (Annex VI to CLP, ATP 23).
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References

- [1] EP and Council. Reg.(EC) No 1907/2006 (REACH). Art.31, Annex II. OJ EU L 396/2006.
- [2] European Commission. Reg.(EU) 2020/878 — amending Annex II REACH. OJ EU L 203/2020. From 01.01.2023.
- [3] EP and Council. Reg.(EC) 1272/2008 (CLP) + ATP 23. OJ EU L 353/2008.
- [4] United Nations. GHS Rev.9. ST/SG/AC.10/30/Rev.9. ONZ, 2021.
- [5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs.
- [6] ISO. ISO 3864-1:2011 — Safety colours and safety signs.
- [7] Act of 26.06.1974 — Labour Code (Poland). Art.221-229. Journal of Laws 2023 item 1465.
- [8] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=58-85-5>

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL857

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Generator: Document prepared automatically on the basis of the ECHA harmonised classification (Annex VI to CLP, ATP 23) and public physico-chemical databases.

Author: www.MolGod.org — automated safety data sheet (SDS) platform.

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