SAFETY DATA SHEET (SDS)

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

Date: 18.10.2026 | Version: 4 | EN

2-(((Dodecylsulfanyl)carbonothioyl)sulfanyl)-2-methylpropanoic acid

2-dodecylsulfanylcarbothioylsulfanyl-2-methylpropanoic acid

CAS 461642-78-4

$C_{17}H_{32}O_2S_3$ | EC 663-505-0

MOLAR MASS	LOGP	TPSA
364.60	8	120 Å²

HAZARD CLASSIFICATION (GHS / CLP)

CLP classification not established — no harmonised entry (Annex VI), and the provenance of the self-classification has not been established. Verification in the ECHA C&L inventory / the manufacturer's safety data sheet is required. Do NOT assume the absence of hazard.

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

1.1 Substance name	2-(((Dodecylsulfanyl)carbonothioyl)sulfanyl)-2-methylpropanoic acid
1.1 IUPAC name	2-dodecylsulfanylcarbothioylsulfanyl-2-methylpropanoic acid
1.1 CAS number	461642-78-4
1.1 EC number	663-505-0
1.1 PubChem CID	11473994
1.1 InChIKey	DZFGVGDQHQHOKZ-UHFFFAOYSA-N
1.1 SMILES	CCCCCCCCCCCCSC(=S)SC(C)(C)C(=O)O
1.1 Molecular formula	$C_{17}H_{32}O_2S_3$ [7]
1.1 Molar mass	364.6 g/mol [7]
1.1 Exact mass	364.1564 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

CLP classification not established — no harmonised entry (Annex VI), and the provenance of the self-classification has not been established. Verification in the ECHA C&L inventory / the manufacturer's safety data sheet is required. Do NOT assume the absence of hazard.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	461642-78-4
EC number	663-505-0
Molecular formula	$C_{17}H_{32}O_2S_3$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)

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]

Skin contact

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

Eye contact

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

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]

Symptoms and effects

No specific symptoms described in the literature. [1][2]

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, SOx.
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. [1][2]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2]
Methods for containment and cleaning up	Absorb with inert material (sand, vermiculite, diatomaceous earth) and collect into sealed, labelled containers. Do not release into drains. [1][2]
Related sections	8; 13

WORKING DRAFT 工作草案

7. Handling and storage

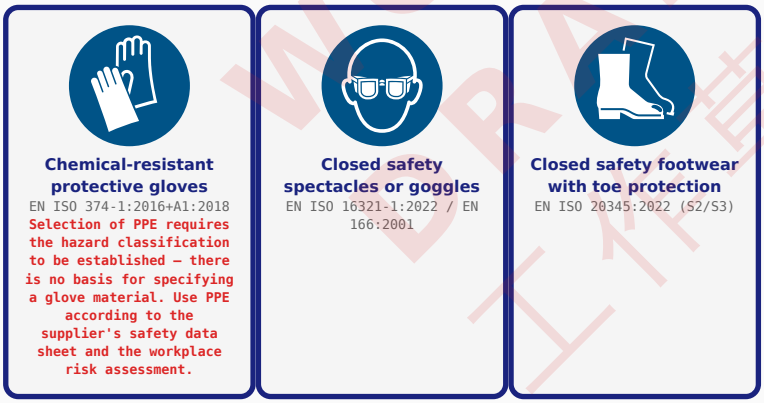
Precautions	Work in a fume hood or with adequate ventilation. No eating, drinking or smoking in the work area. [1][2]
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. [1][2]
Humidity	Store in a dry place (<60% RH). [1][2]
Light	Protect from direct sunlight. [1][2]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

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)



Chemical-resistant protective gloves
EN ISO 374-1:2016+A1:2018
Selection of PPE requires the hazard classification to be established — there is no basis for specifying a glove material. Use PPE according to the supplier's safety data sheet and the workplace risk assessment.

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	No data available.	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	No data available.	
Boiling point	No data available.	
Flash point	No data available.	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	No data available.	

WORKING DRAFT 工作草稿

Property (item 9.1)	Value	Source
Vapour pressure	No data available.	
Relative vapour density	No data available.	
Kinematic viscosity	No data available.	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Water solubility	No data available.	
Particle characteristics	No data available.	
Partition coefficient n-octanol/water (log value)	8 [8]	
Molar mass	364.6 g/mol [7] ✓86%	*PubChem*
Molecular formula	$C_{17}H_{32}O_2S_3$ [7] ✓86%	*PubChem*
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, strong bases, Base metals (hydrogen evolution).
Decomposition products	Thermal decomposition products: CO, CO2, SOx.

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.

WORKING DRAFT 工作草案

12. Ecological information

Aquatic toxicity	No data available.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 8 [8]. Elevated bioaccumulation potential (log Kow ≥ 4.5 — PBT/vPvB screening threshold per ECHA R.11); a definitive assessment requires the bioconcentration factor BCF (REACH Annex XIII: B if BCF > 2000). [10][11]
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)	The waste code (EWC) cannot be determined without a hazard classification — the provenance of the classification has not been established. Do NOT assume either hazardousness (16 05 06*) or the absence thereof (16 05 09); determine it after verifying the classification in ECHA. [9]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be handled in accordance with the waste classification (see the EWC code above); where no classification has been established, do not assume the absence of hazard.

14. Transport information

UN number	VERIFICATION REQUIRED — no verified UN assignment.
Environmental hazard	Environmental hazard for transport: not verified. Classification provenance undetermined — do NOT assume absence of environmental hazard or that marine pollutant marking is not required; verify against CLP Annex VI, Section 12 and ADR 2.2.9 / IMDG criteria before shipping.
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.

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]

16. Other information

Legal status of classification: provenance not recorded — requires verification in ECHA.Entries with an entry-into-force date after 17.10.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

Madan Kapre. *Chapter-78 Nodule of Zuckerkandl*. Atlas of Thyroid Surgery (2013). DOI: 10.5005/jp/books/12026_127

78. Musing (2011). DOI: 10.15215/aupress/9781897425909.079

78. Bibliothek - Forschung und Praxis (2004). DOI: 10.1515/9783110951929.bm

DISTINGUISHED. Scald DOI: 10.2307/j.ctt1mtz5fq.27

WORKING DRAFT · 工作草案

Chains. Interstate DOI: 10.2307/j.ctt16nzfh0.59

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

v4 (17.10.2026)	Classification provenance not recorded in the canon — verify the source in ECHA (Annex VI / C&L).

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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[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: 2026-10-17.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-17.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-17.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/11473994

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

[9] 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

[10] 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

[11] 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

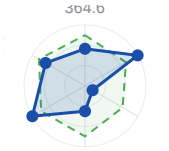
[12] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-10-17.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=461642-78-4

WORKING DRAFT · 工作草案

ADMET / Drug-likeness



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 classification of unrecorded provenance (to be verified in ECHA) and public physicochemical databases.
Author: www.MolGod.org — platform for automated safety data sheets (SDS).
Issue date: 18.10.2026 | Document version: 4

WORKING DRAFT · 工作草案