

SAFETY DATA SHEET (SDS)

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

Date: 03.09.2026 | Version: 1 | EN

N-[3-[(3-amino-3-oxoprop-1-en-2-yl)amino]-3-oxoprop-1-en-2-yl]-2-[(11E)-37-butan-2-yl-18-(2,3-dihydroxybutan-2-yl)-11-ethylidene-59-hydroxy-8,31-bis(1-hydroxyethyl)-26,40,46-trimethyl-43-methylidene-6,9,16,23,28,38,41,44,47-nonaoxo-27-oxa-3,13,20,56-tetrathia-7,10,17,24,36,39,42,45,48,52,58,61,62,63,64-pentadecazanonacyclo[23.23.9.329,35.12,5.112,15.119,22.154,57.01,53.032,60]tetrahexaconta-2(64),4,12(63),19(62),21,29(61),30,32(60),33,51,54,57-dodecaen-51-yl]-1,3-thiazole-4-carboxamide

N-[3-[(3-amino-3-oxoprop-1-en-2-yl)amino]-3-oxoprop-1-en-2-yl]-2-[(11E)-37-butan-2-yl-18-(2,3-dihydroxybutan-2-yl)-11-ethylidene-59-hydroxy-8,31-bis(1-hydroxyethyl)-26,40,46-trimethyl-43-methylidene-6,9,16,23,28,38,41,44,47-nonaoxo-27-oxa-3,13,20,56-tetrathia-7,10,17,24,36,39,42,45,48,52,58,61,62,63,64-pentadecazanonacyclo[23.23.9.329,35.12,5.112,15.119,22.154,57.01,53.032,60]tetrahexaconta-2(64),4,12(63),19(62),21,29(61),30,32(60),33,51,54,57-dodecaen-51-yl]-1,3-thiazole-4-carboxamide

CAS 1393-48-2 $C_{72}H_{85}N_{19}O_{18}S_5$ **EC 215-734-9**

HAZARD CLASSIFICATION (GHS / CLP)

**Warning****H302**

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

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

1.1 Substance name

—

1.1 IUPAC name

N-[3-[(3-amino-3-oxoprop-1-en-2-yl)amino]-3-oxoprop-1-en-2-yl]-2-[(11E)-37-butan-2-yl-18-(2,3-dihydroxybutan-2-yl)-11-ethylidene-59-hydroxy-8,31-bis(1-hydroxyethyl)-26,40,46-trimethyl-43-methylidene-6,9,16,23,28,38,41,44,47-nonaoxo-27-oxa-3,13,20,56-tetrathia-7,10,17,24,36,39,42,45,48,52,58,61,62,63,64-pentadecazanonacyclo[23.23.9.329,35.12,5.112,15.119,22.154,57.01,53.032,60]tetrahexaconta-2(64),4,12(63),19(62),21,29(61),30,32(60),33,51,54,57-dodecaen-51-yl]-1,3-thiazole-4-carboxamide

1.1 CAS number

1393-48-2

1.1 EC number

215-734-9

1.1 PubChem CID

16129666

1.1 InChIKey

NSFFHOGKXHRQEW-DVRIZHICSA-N

1.1 SMILES

CCC(C)C1C(=O)NC(C(=O)NC(=C)C(=O)NC(C(=O)NC23CCC(=NC2C4=CSC(=N4)C(C(OC(=O)C5=NC6=C(C=CC(C6O)N1)C(=C)O)C(=C)C)NC(=O)C(NC(=O)C9=CSC3=N9)C(C(O)C(C(C(O)O)C1=NC(=C51)C(=O)NC(=C)C(=O)NC(=C)C(=O)N)C

1.1 Molecular formula

 $C_{72}H_{85}N_{19}O_{18}S_5$ ^[7]

1.1 Molar mass

1664.9 g/mol ^[7]

1.1 Exact mass

1663.4924 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 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.
SUPPLIER DETAILS — NOT FOR
DISTRIBUTION MolGod.org prepares documentation and is not the supplier of this substance.

1.4 Emergency telephone number

Emergency telephone 112 (EU-wide emergency number)

The number above is the Polish poison centre (CIT, Lodz, 24/7). It is NOT the poison centre designated for your country. Under Article 45 of Regulation (EC) No 1272/2008 the competent body is the centre designated in the country of placing on the market — consult it before use.

2. Hazards identification

GHS:



PPE:



Prohibitions:



Warning

Hazard statements (H) [3][4]

H302 Harmful if swallowed

Precautionary statements (P) [3][4]

P264 Wash thoroughly after handling
P270 Do not eat, drink or smoke when using this product
P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P330 Rinse mouth
P501 Dispose of contents/container to an approved waste collection point

Non-harmonised classification (no entry in Annex VI to CLP) — assigned from aggregated ECHA C&L notifications; the H-statements require verification against the official source (ECHA C&L / manufacturer's data sheet).

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	1393-48-2
EC number	215-734-9
Molecular formula	C ₇₂ H ₈₅ N ₁₉ O ₁₈ S ₅
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][10]}

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). ^{[1][2][10]}

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. ^{[1][2][10]}

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 42 631 47 24 (24/7). Emergency number: 112. ^{[1][2][10]}

Symptoms and effects

nausea, vomiting, diarrhoea. ^[3]

Notes for physician

Requires verification

Emergency numbers: CIT Łódź: +48 42 631 47 24 (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 . ^[11]
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][10]}
Environmental precautions	Prevent entry into sewers, groundwater and surface water. ^{[1][2][10]}
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][10]}
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. ^{[1][2][10]}
Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. ^{[1][2][10]}
Humidity	Store in a dry place (<60% RH). ^{[1][2][10]}

Light	Protect from direct sunlight. ^{[1][2][10]}
Incompatible materials	Strong oxidizers. ^[11]

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][12]}

 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)
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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.	
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	
Rozpuszcz. w wodzie	No data available.	
Particle characteristics	No data available.	

Property (item 9.1)	Value	Source
Partition coefficient n-octanol/water (log value)	0.6 ^[8]	
Molar mass	1664.9 g/mol ^[7]	
Molecular formula	C ₇₂ H ₈₅ N ₁₉ O ₁₈ S ₅ ^[7]	
Lipinski rule (RO5)	FAIL	

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	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	log Kow = 0.6 ^[8] . Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). ^{[13][14]}
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 (np. chemical reagents) zawierające substancje niebezpieczne. EWC code verification required. ^[9]
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	Environmental hazard for transport: not verified. Non-harmonised classification (outside CLP Annex VI) — verify aquatic toxicity (Section 12) and do NOT assume marine pollutant marking is not required; confirm per ADR 2.2.9 / IMDG 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: supplier self-classification under Art. 4(3) CLP — no harmonised entry in Annex VI. Entries with an entry-into-force date after 03.09.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

- Zhang Y, Yi R, Zhou X et al.. ALDH1L2 induces resistance to chemotherapy in small cell lung cancer by inhibiting ferroptosis.. Redox biology (2026). DOI: 10.1016/j.redox.2026.104098
- Silva L, Almeida L, Al-Naimi F et al.. The Streptomyces Metabolite Thiostrepton Inhibits Regulatory T Cell Differentiation and Function to Boost Antitumor Immune Responses.. European journal of immunology (2025). DOI: 10.1002/eji.70035
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- Khan AQ, Agha M, Ahmad F et al.. Targeting FOXM1 regulates metabolic signatures through ROS-dependent JNK/Bmi1/Skp2 axis in human cutaneous T-cell lymphoma.. Cell death & disease (2026). DOI: 10.1038/s41419-025-08389-z
- Gibson V, Dzialo J, Messier T et al.. Preclinical characterization and phase 1 clinical testing of targeting mitochondrial peroxiredoxin 3 in cancer.. Nature communications (2026). DOI: 10.1038/s41467-026-75153-y

Safety Data Sheet (SDS) — N-[3-[(3-amino-3-oxoprop-1-en-2-yl)amino]-3-oxoprop-1-en-2-yl]-2-[(11E)-3,7-butan-2-yl-18-(2,3-dihydroxybutan-2-yl)-11-ethylidene-59-hydroxy-8,31-bis(1-hydroxyethyl)-26,40,46-trimethyl-43-methylidene-6,9,16,23,28,38,41,44,47-nonadeca-27-oxa-3,13,20,56-tetrathia-7,10,17,24,36,39,42,45,48,52,58,61,62,63,64-pentadecazanonacyclo[23.23.9.329.35.12.5.112.15.119.22.154.57.01.53.032.60]tetrahexaconta-2(64),4,12(63),19(62),21,29(61),30,32(60),33,51,54,57-dodecaen-51-yl]-1,3-thiazole-4-carboxamide · CAS 1202 49 2

Full text of H statements

H302 Harmful if swallowed

Full text of P statements

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P270 Do not eat, drink or smoke when using this product

P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

P330 Rinse mouth

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)

STOT Specific Target Organ Toxicity

SVHC Substance of Very High Concern

TPSA Topological Polar Surface Area

vPvB very Persistent and very Bioaccumulative

Version history

v1 (03.09.2026) Based on supplier self-classification (ECHA C&L notifications; no harmonised entry in Annex VI).

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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [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: 2026-09-03.
- [5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: <https://www.iso.org/standard/72424.html> Accessed: 2026-09-03.
- [6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: <https://www.iso.org/standard/51021.html> Accessed: 2026-09-03.
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- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/16129666>
- [8] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: <https://hbcpc.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] 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
- [11] Urban, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.
- [12] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.
- [13] 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>
- [14] 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>
- [15] 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: 2026-09-03.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=1393-48-2>

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



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