

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

3,6,9,12-tetra-azatetradecamethylenediamine;
pentacthylenehexamine

N'-[2-[2-[2-(2-aminoethylamino)ethylamino]ethylamino]ethyl]ethane-1,2-diamine

CAS 4067-16-7

 $C_{10}H_{28}N_6$

EC 223-775-9

MOLAR MASS
232.37LOGP
-3.4

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H314

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	3,6,9,12-tetra-azatetradecamethylenediamine; pentacthylenehexamine
1.1 IUPAC name	N'-[2-[2-[2-(2-aminoethylamino)ethylamino]ethylamino]ethyl]ethane-1,2-diamine
1.1 CAS number	4067-16-7
1.1 EC number	223-775-9
1.1 PubChem CID	19990
1.1 InChIKey	LSHROXHEILXKHM-UHFFFAOYSA-N
1.1 SMILES	C(CNCCNCCNCCNCCN)N
1.1 Molecular formula	$C_{10}H_{28}N_6$ ^[7]
1.1 Molar mass	232.37 g/mol ^[7]
1.1 Exact mass	232.2375 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)

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



Danger

Hazard statements (H) [3][4][9]

H314	Causes severe skin burns and eye damage
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][9]

P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
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
P301+P330+P331	IF SWALLOWED: Rinse mouth; Do NOT induce vomiting
P302+P352	IF ON SKIN: Wash with plenty of water
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing; Rinse skin with water or shower
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
P310	Immediately call a POISON CENTER or doctor/physician
P321	Specific treatment
P333+P313	If skin irritation or rash occurs: Get medical advice/attention
P362+P364	Take off contaminated clothing
P363	Wash contaminated clothing before reuse
P391	Collect spillage
P405	Store locked up
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.

3. Composition/information on ingredients

Substance type	pure substance
CAS Number	4067-16-7
EC number	223-775-9
Molecular formula	$C_{10}H_{28}N_6$
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	612-064-00-2

4. First aid measures



Inhalation

Move the affected person to fresh air. Keep at rest. If not breathing: artificial respiration (qualified personnel only). [\[1\]](#)[\[2\]](#)[\[11\]](#)

Skin contact

Remove contaminated clothing. Rinse skin with soap and water (min. 15 minutes). Call a physician immediately. [\[1\]](#)[\[2\]](#)[\[11\]](#)

Eye contact

Rinse eyes with running water (min. 15 minutes). Remove contact lenses if possible. If irritation persists — consult an ophthalmologist. [\[1\]](#)[\[2\]](#)[\[11\]](#)

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. [\[1\]](#)[\[2\]](#)[\[11\]](#)

Symptoms and effects

skin redness and irritation. [\[3\]](#)[\[9\]](#)

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 . [12]
Advice for firefighters	Use self-contained breathing apparatus (SCBA). Full protective suit.
Flash Point	93.3°C [7]
Auto-ignition temperature	360°C [7]

6. Accidental release measures

Personal precautions	Use personal protective equipment (see Section 8). Avoid breathing dust/vapours. [1] [2] [11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1] [2] [11]
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] [11]
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] [11]
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Storage temperature	Store at room temperature (15-25°C) or as indicated on the label. ^{[1][2][11]}
Humidity	Store in a dry place (<60% RH). ^{[1][2][11]}
Light	Protect from direct sunlight. ^{[1][2][11]}
Incompatible materials	Strong oxidizers. ^[12]

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][13]}

 Chemical-resistant protective gloves EN ISO 374-1:2016+A1:2018 butyl (type B/C) – NOT latex	 Closed safety spectacles or goggles EN ISO 16321-1:2022 / EN 166:2001	 Face shield (splash risk) EN ISO 16321-1:2022	 Chemical-resistant protective clothing EN 13034:2005+A1:2009 (typ 6) / EN 14126:2003 (bio)	 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	93.3°C (experimental data) ^[7]	
Flammability	No data available.	
Lower and upper explosion limit	No data available.	
Density (20°C)	1 g/cm ³ ^[7]	
Vapour pressure	No data available.	
Relative vapour density	No data available.	
Kinematic viscosity	No data available.	
Auto-ignition temperature	360°C (experimental data) ^[7]	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	No data available.	

Property (item 9.1)	Value	Source
Particle characteristics	No data available.	
Partition coefficient n-octanol/water (log value)	-3.4 ^[8]	
Molar mass	232.37 g/mol ^[7]	
Molecular formula	C ₁₀ H ₂₈ N ₆ ^[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, CO ₂ , NO _x .

11. Toxicological information

LD50 (oral)	No data available.
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Category 1 (H314) — corrosive; sub-category (1A/1B/1C) per CLP Annex VI entry. ^{[3][9]}
Eye irritation	Serious eye damage — covered by the corrosive classification (H314; CLP Annex I 3.3.2.1). ^{[3][9]}
Sensitisation	Skin, Category 1 (H317): May cause an allergic skin reaction. ^{[3][9]}
Mutagenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
Carcinogenicity	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
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	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
STOT — single exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
STOT — repeated exposure	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
Aspiration hazard	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}

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). Numerical LC ₅₀ /EC ₅₀ data unverified in the available dataset — do not assume absence of toxicity.(M-factor for acute/chronic cat. 1 — to be verified per Table 3 of Annex VI, if assigned.)
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = -3.4 ^[8] . Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). ^{[14][15]}
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. ^[10]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 8 — Corrosive substances

UN number	UN 2735 ^[7]
Transport hazard class	Suggested from GHS classification — VERIFICATION REQUIRED.
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	UN number per the indicated source. Verify the transport class and packing group in ADR Table A / UN Model Regulations before shipment. ^[7]
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]

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 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)

Jon M. Peha. Cellular Competition and the Weighted Spectrum Screen. (2013). DOI: 10.2139/ssrn.2241276

Sanaa Ismail, Ricardo Amaral, Attia A. Gadallah et al.. Machine-learning screening and first-principles lattice dynamics resolve the most stable structure of NaCa(BH₄)₃ from a data-driven candidate search. arXiv (2609.02001v1) (2026).

Avaneesh Balasubramanian, Gopalakrishnan Sai Gautam. Extending the Pnictide Chemical Space for Photovoltaics. arXiv (2608.30402v1) (2026).

Jian-Feng Zhang, Sheng Xu, Zhong-Yi Lu et al.. Symmetry-Preserving Phase Transitions in AM_2Al_9 Materials under Pressure. arXiv (2608.28957v1) (2026).

Balaka Mondal, D. Thirumalai. Persistence length of short homopolymeric single-stranded DNA sequences in polyvalent cations. arXiv (2608.25046v1) (2026).

Full text of H statements

H314	Causes severe skin burns and eye damage
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

P260	Do not breathe dust/fume/gas/mist/vapours/spray
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P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes; Remove contact lenses, if present and easy to do. Continue rinsing
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P333+P313	If skin irritation or rash occurs: Get medical advice/attention
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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 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: 2026-09-03.
- [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.
- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/19990>
- [8] Rumble, J.R., ed. CRC Handbook of Chemistry and Physics. 105th ed. Boca Raton: CRC Press, 2024. URL: <https://hbcpc.chemnetbase.com>
- [9] ECHA. European Chemicals Agency — harmonised classification inventory (CLP Annex VI). URL: <https://echa.europa.eu>
- [10] 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>
- [11] 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
- [12] Urben, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.
- [13] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.
- [14] 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>
- [15] 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>
- [16] 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=4067-16-7>
ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL65184

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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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).

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