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SAFETY DATA SHEET (SDS)

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

Date: 18.10.2026 | Version: 5 | EN

Dimethylhexadecylamine

N,N-dimethylhexadecan-1-amine

CAS 112-69-6

$C_{18}H_{39}N$ | EC 203-997-2

MOLAR MASS	LOGP
269.50	8

TPSA: 3.2 Å²

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H302 | H314 | H400 | H335

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	Dimethylhexadecylamine
1.1 IUPAC name	N,N-dimethylhexadecan-1-amine
1.1 CAS number	112-69-6
1.1 EC number	203-997-2
1.1 PubChem CID	16221
1.1 InChIKey	NHLUVTZJQOJKCC-UHFFFAOYSA-N
1.1 SMILES	CCCCCCCCCCCCCCCCN(C)C
1.1 Molecular formula	$C_{18}H_{39}N$ [7]
1.1 Molar mass	269.5 g/mol [7]
1.1 Exact mass	269.3083 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:



Prohibitions:



Danger

Hazard statements (H) [3][4]

H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H400	Very toxic to aquatic life
H335	May cause respiratory irritation

Precautionary statements (P) [3][4]

P260	Do not breathe dust/fume/gas/mist/vapours/spray
P264	Wash thoroughly after handling
P270	Do not eat, drink or smoke when using this product
P271	Use only outdoors or in a well-ventilated area
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P301+P330+P331	IF SWALLOWED: Rinse mouth; Do NOT induce vomiting
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
P312	Call a POISON CENTER or doctor/physician if you feel unwell
P321	Specific treatment
P330	Rinse mouth
P363	Wash contaminated clothing before reuse
P391	Collect spillage
P403+P233	Store in a well-ventilated place: Keep container tightly closed
P405	Store locked up
P501	Dispose of contents/container to an approved waste collection point

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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	112-69-6
EC number	203-997-2
Molecular formula	$C_{18}H_{39}N$
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][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. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][11]

Symptoms and effects

nausea, vomiting, diarrhoea; cough, shortness of breath, headache, dizziness; skin redness and irritation. [3]

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. [12]
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 vapours. [1][2][11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][11]
Methods for containment and cleaning up	Contain the spill with a barrier. Absorb with inert material (sand, vermiculite, diatomaceous earth). Collect into sealed, labelled containers. Do not release into drains. [1][2][11]
Related sections	8; 13

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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]
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]



9. Physical and chemical properties

NOTE: The substance may solidify below 12.0°C.

Property (item 9.1)	Value	Source
Physical state	Liquid	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	12°C [8] ✓86%	*NIST WebBook + source consensus*
Boiling point	No data available.	
Flash point	No data available.	
Flammability	No data available.	

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Property (item 9.1)	Value	Source
Lower and upper explosion limit	No data available.	
Density (20°C)	No data available.	
Vapour pressure	No data available.	
Relative vapour density	9.30 [16]	
Kinematic viscosity	No data available.	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Water solubility	No data available.	
Particle characteristics	Not applicable (REACH 9.1(r))	
Partition coefficient n-octanol/water (log value)	8 [9]	
Molar mass	269.5 g/mol [7] ✓86%	*PubChem*
Molecular formula	$C_{18}H_{39}N$ [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.
Decomposition products	Thermal decomposition products: CO, CO2, NOx.

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 supplier self-classification (no harmonised Annex VI entry). [3]
Eye irritation	Serious eye damage — covered by the corrosive classification (H314; CLP Annex I 3.3.2.1). [3]
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	Category 3 (H335): May cause respiratory irritation. [3]
STOT — repeated exposure	No data available.
Aspiration hazard	No data available.

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12. Ecological information

Aquatic toxicity	Classification per ECHA C&L notifications (self-classification, Art. 4(3)): H400 — Very toxic to aquatic life (Aquatic Acute 1). Numerical LC_{50}/EC_{50} data unverified in the available dataset — do not assume absence of toxicity.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 8 [9]. 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). [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 (e.g. chemical reagents) containing hazardous substances. Verification of the EWC code 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) 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]

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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 18.10.2026 were omitted as future (not yet applicable).

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

Full text of H statements

H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H400	Very toxic to aquatic life
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Full text of P statements

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P330	Rinse mouth
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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

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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

v5 (18.10.2026)	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: 2026-10-18.

[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: 2026-10-18.

[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: 2026-10-18.

[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: 2026-10-18.

[5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: https://www.iso.org/standard/72424.html Accessed: 2026-10-18.

[6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: https://www.iso.org/standard/51021.html Accessed: 2026-10-18.

[7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: https://pubchem.ncbi.nlm.nih.gov/compound/16221

[8] NIST. Chemistry WebBook, SRD 69. National Institute of Standards and Technology. URL: https://webbook.nist.gov/cgi/cbook.cgi?ID=112-69-6

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

[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] MOL-GOD. Value obtained by calculation from the molecular formula/molecular weight (the specific quantity and its formula are indicated at the respective field). Calculated value, not an experimental measurement. URL: https://www.nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses

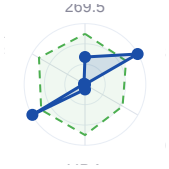
[17] MRiPS Regulation of 12.06.2018 — NDS/NDN. Journal of Laws 2024 item 1017. URL: https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20240001017 Accessed: 2026-10-18.

External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=112-69-6

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1877748

ADMET / Drug-likeness



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