

SAFETY DATA SHEET (SDS)

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

Date: 02.09.2026 | Version: 1 | EN

pentaerythritol dibromide

2,2-bis(bromomethyl)propane-1,3-diol

CAS 3296-90-0

 $C_5H_{10}Br_2O_2$

EC 221-967-7

MOLAR MASS
261.94LOGP
0.5

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H350 H340

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	pentaerythritol dibromide
1.1 IUPAC name	2,2-bis(bromomethyl)propane-1,3-diol
1.1 CAS number	3296-90-0
1.1 EC number	221-967-7
1.1 PubChem CID	18692
1.1 InChIKey	CHUGKEQJSLOLHL-UHFFFAOYSA-N
1.1 SMILES	<chem>C(C(CO)(CBr)CBr)O</chem>
1.1 Molecular formula	$C_5H_{10}Br_2O_2$ ^[7]
1.1 Molar mass	261.94 g/mol ^[7]
1.1 Exact mass	261.9027 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)

2. Hazards identification

GHS:



PPE:



Danger

Hazard statements (H) ^{[3][4][9]}

H350	May cause cancer
H340	May cause genetic defects

Precautionary statements (P) ^{[3][4][9]}

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P280	Wear protective gloves/protective clothing/eye protection/face protection
P308+P313	IF exposed or concerned: Get medical advice/attention
P405	Store locked up
P501	Dispose of contents/container to an approved waste collection point

NOTE: CMR substance — employment of pregnant and breastfeeding women in work harmful to health is prohibited (Polish Labour Code Art. 176 § 1; Council of Ministers Regulation of 3 April 2017, Journal of Laws 2017 item 796). ^{[13][14]}

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	3296-90-0
EC number	221-967-7
Molecular formula	C ₅ H ₁₀ Br ₂ O ₂
Concentration	≥99% (typical reagent-grade purity — to be confirmed by the supplier's specification)
Clp index no	603-240-00-X

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

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

No specific symptoms described in the literature. [\[3\]](#)[\[9\]](#)

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 , HBr. [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 dust. [1] [2] [11]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1] [2] [11]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [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]
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][15]}

 Chemical-resistant protective gloves EN ISO 374-1:2016+A1:2018 fluoroelastomer FKM (Viton), min. 0.4 mm — NOT nitrile (breakthrough within minutes)	 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	Solid	
Colour	No data available.	
Odour	No data available.	
pH (1% aqueous solution)	No data available.	
Melting point	113°C (experimental data) ^[7]	
Boiling point	No data available.	
Flash point	Not applicable (REACH 9.1(h))	
Flammability	No data available.	
Lower and upper explosion limit	Not applicable (REACH 9.1(g))	
Density (20°C)	2.2 g/cm ³ ^[7]	
Vapour pressure	0 kPa (0.000013 mmHg) (experimental data) ^[7]	
Relative vapour density	Not applicable (REACH 9.1(q))	
Kinematic viscosity	Not applicable (REACH 9.1(l))	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Rozpuszcz. w wodzie	38 g/L, 25°C ^[7]	

Property (item 9.1)	Value	Source
Particle characteristics	The particle size distribution has not been determined for this commercial form – required under Annex II 9.1(r); to be completed from the supplier's specification.	
Partition coefficient n-octanol/water (log value)	0.5 ^[8]	
Molar mass	261.94 g/mol ^[7]	
Molecular formula	C ₅ H ₁₀ Br ₂ O ₂ ^[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 , HBr.

11. Toxicological information

LD50 (oral)	LD50 3458 mg/kg (rat, oral) ^[7]
LD50 (dermal)	No data available.
LC50 (inhalation)	No data available.
Skin irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
Eye irritation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
Sensitisation	Not classified for this hazard (outside the scope of the harmonised classification in CLP Annex VI; verify supplier self-classification) ^{[3][9]}
Mutagenicity	Category 1A/1B (harmonised classification, Annex VI to CLP).
Carcinogenicity	Category 1A/1B (harmonised classification, Annex VI to CLP).
IARC classification (carcinogenicity)	IARC Group 2B — possibly carcinogenic to humans. [local snapshot — not verified against the current IARC list] ^[18]
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	No data available.
Persistence / biodegradability	No data available.
Bioaccumulative potential	log Kow = 0.5 ^[8] . Low bioaccumulation potential (log Kow < 4.5 — PBT/vPvB screening criterion per ECHA Guidance R.11). ^{[16][17]}
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

UN number	VERIFICATION REQUIRED — no verified UN assignment.
Environmental hazard	Not classified as environmentally hazardous for transport (no H400/H410/H411 in CLP Annex VI; no marine pollutant mark required) ^[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	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	Subject to general entries 28–30 of REACH Annex XVII (CMR substance cat. 1A/1B): sale to the general public prohibited — supply to professional users only. ^[1]
IARC classification (carcinogenicity)	IARC Group 2B — possibly carcinogenic to humans.

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 02.09.2026 were omitted as future (not yet applicable).

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

Scientific citations (10)

- NTP Toxicology and Carcinogenesis Studies of 2,2-Bis(Bromomethyl)-1,3-Propanediol (FR-1138(R)) (CAS No. 3296-90-0) in F344 Rats and B6C3F1 Mice (Feed Studies).. (1996).
- Dmitriy Melnikov, Guinevere Strack, Marcos Pita et al.. Analog Noise Reduction in Enzymatic Logic Gates. arXiv (0905.2714v1) (2009). DOI: 10.1021/jp904585x
- Zhiwen Zeng, Dezhou Guo, Tao Wang et al.. Chemisorption Induced Formation of Biphenylene Dimer on Surfaces. arXiv (2309.05341v1) (2023). DOI: 10.1021/jacs.1c08284
- Mostafa Abedi, Gianluca Levi, Diana B. Zederkof et al.. Excited-State Solvation Structure of Transition Metal Complexes from Molecular Dynamics Simulations and Assessment of Partial Atomic Charge Methods. arXiv (1812.09090v1) (2018). DOI: 10.1039/c8cp06567e
- NTP carcinogenesis studies of 2,2-bis(bromomethyl)-1,3-propanediol, nitromethane, and 1,2,3-trichloropropane (cas nos. 3296-90-0, 75-52-5, and 96-18-4) in guppies (Poecilia reticulata) and medaka (Oryzias latipes) (Waterborne Studies).. (2005).

Full text of H statements

H350	May cause cancer
H340	May cause genetic defects

Full text of P statements

P201	Obtain special instructions before use
P202	Do not handle until all safety precautions have been read and understood
P280	Wear protective gloves/protective clothing/eye protection/face protection
P308+P313	IF exposed or concerned: Get medical advice/attention
P405	Store locked up
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 (02.09.2026)	Based on 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. URL: <https://eur-lex.europa.eu/eli/reg/2006/1907/oj> Accessed: 2026-09-02.
- [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: 2026-09-02.
- [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: 2026-09-02.
- [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: 2026-09-02.

- [5] ISO. ISO 7010:2019 — Graphical symbols. Safety signs. URL: <https://www.iso.org/standard/72424.html> Accessed: 2026-09-02.
- [6] ISO. ISO 3864-1:2011 — Safety colours and safety signs. URL: <https://www.iso.org/standard/51021.html> Accessed: 2026-09-02.
- [7] PubChem. National Center for Biotechnology Information (NIH/NLM), chemical compound database. URL: <https://pubchem.ncbi.nlm.nih.gov/compound/18692>
- [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] Urban, P.G., ed. Bretherick's Handbook of Reactive Chemical Hazards. 8th ed. Oxford: Academic Press.
- [13] Act of 26 June 1974 — Labour Code (Poland), Art. 176 § 1. Journal of Laws 2023 item 1465. URL: <https://isap.sejm.gov.pl>
- [14] Council of Ministers of the Republic of Poland. Regulation of 3 April 2017 on the list of arduous, hazardous or health-harmful work for pregnant and breastfeeding women. Journal of Laws 2017 item 796. URL: <https://isap.sejm.gov.pl/isap.nsf/DocDetails.xsp?id=WDU20170000796>
- [15] CEN. Personal protective equipment standards (EN ISO 374-1, EN 166, EN 149, EN 14387, EN ISO 20345). Brussels: European Committee for Standardization.
- [16] 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>
- [17] 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>
- [18] IARC. IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. Lyon: International Agency for Research on Cancer. URL: <https://monographs.iarc.who.int>
- [19] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: <https://cfpub.epa.gov/ecotox/>
- [20] 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: 2026-09-02.

External links

NIST: <https://webbook.nist.gov/cgi/cbook.cgi?ID=3296-90-0>
 Wikidata: <https://www.wikidata.org/wiki/Q26841193>
 ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL1407005

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

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