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

Benzethonium Chloride

benzyl-dimethyl-[2-[2-[4-(2,4,4-trimethylpentan-2-yl)phenoxy]ethoxy]ethyl]azanium chloride

CAS 121-54-0

$C_{27}H_{42}ClNO_2$ | EC 204-479-9

MOLAR MASS	TPSA
448.10	18.5 Å²

HAZARD CLASSIFICATION (GHS / CLP)



Danger

H301 | H314 | H400 | H410 | H302 | H315 | H319

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	Benzethonium Chloride
1.1 IUPAC name	benzyl-dimethyl-[2-[2-[4-(2,4,4-trimethylpentan-2-yl)phenoxy]ethoxy]ethyl]azanium chloride
1.1 CAS number	121-54-0
1.1 EC number	204-479-9
1.1 PubChem CID	8478
1.1 InChIKey	UREZNYTWGJKWBI-UHFFFAOYSA-M
1.1 SMILES	CC(C)(C)CC(C)(C)C1=CC=C(C=C1)OCCOCC[N+](C)(C)CC2=CC=CC=C2.[Cl-]
1.1 Molecular formula	$C_{27}H_{42}ClNO_2$ [7]
1.1 Molar mass	448.1 g/mol [7]
1.1 Exact mass	447.2904 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]

H301	Toxic if swallowed
H314	Causes severe skin burns and eye damage
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye 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
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
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
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
P330	Rinse mouth
P332+P313	If skin irritation occurs: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention

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P363	Wash contaminated clothing before reuse
P391	Collect spillage
P405	Store locked up
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	121-54-0
EC number	204-479-9
Molecular formula	$C_{27}H_{42}ClNO_2$
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). Call a physician immediately. [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. Emergency number: 112 (EU-wide). Contact the poison centre designated in your country (CLP Art. 45). [1][2][10]

Symptoms and effects

nausea, vomiting, diarrhoea; skin redness and irritation; eye irritation and watering. [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).

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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, HCl (hydrogen chloride). [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. [1][2][10]
Environmental precautions	Prevent entry into sewers, groundwater and surface water. [1][2][10]
Methods for containment and cleaning up	Collect mechanically into suitable containers. Absorption: sand, vermiculite, diatomaceous earth. Do not sweep dry (dust formation). [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
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

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)

9. Physical and chemical properties

Property (item 9.1)	Value	Source
Physical state	Solid	

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Property (item 9.1)	Value	Source
Colour	No data available.	
Odour	Mild odor [7]	
pH (1% aqueous solution)	No data available.	
Melting point	164°C (experimental data) [7]	*PubChem (experimental data)*
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)	No data available.	
Vapour pressure	No data available.	
Relative vapour density	Not applicable (REACH 9.1(q))	
Kinematic viscosity	Not applicable (REACH 9.1(l))	
Refractive index nD^{20}	1.5101 (experimental data) [7]	
Auto-ignition temperature	No data available.	
Decomposition temperature	Not applicable	
Water solubility	No data available.	
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.	
log Kow (XLogP3)	No data available.	
Molar mass	448.1 g/mol [7] ✓86%	*PubChem*
Molecular formula	$C_{27}H_{42}ClNO_2$ [7] ✓86%	*PubChem*

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, HCl (hydrogen chloride).

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	Category 2 — eye irritation.

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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	Classification per ECHA C&L notifications (self-classification, Art. 4(3)): H400 — Very toxic to aquatic life (Aquatic Acute 1); H410 — Very toxic to aquatic life with long lasting effects (Aquatic Chronic 1). LC_{50} (fish): 1.4 mg/L (Lepomis macrochirus, 96 h). EC_{50} (Daphnia): 0.39 mg/L (Daphnia magna, 48 h). EC_{50} (algae): 0.22 mg/L (Raphidocelis subcapitata, 48 h) [13]
Persistence / biodegradability	No data available.
Bioaccumulative potential	No data available.
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. [9]
Packaging	Cleaned packaging may be recycled. Contaminated packaging must be treated as hazardous waste.

14. Transport information



Class 6.1 — Toxic substances



Class 8 — Corrosive substances

UN number	VERIFICATION REQUIRED — no verified UN assignment.
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	NOTE: the GHS classification indicates the substance may be subject to dangerous goods transport regulations (ADR/IMDG/IATA). Do NOT assume absence of restrictions — verify the UN number before shipping.
Environmentally hazardous (mark: fish and tree)	Yes

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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 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

H301	Toxic if swallowed
H314	Causes severe skin burns and eye damage
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye irritation

Full text of P statements

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
P273	Avoid release to the environment
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
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
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
P330	Rinse mouth
P332+P313	If skin irritation occurs: Get medical advice/attention
P337+P313	If eye irritation persists: Get medical advice/attention
P363	Wash contaminated clothing before reuse
P391	Collect spillage
P405	Store locked up

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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
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/8478

[8] ECHA. REACH Registration Dossier (registered substance, acute toxicity study record). Helsinki: European Chemicals Agency. URL: https://echa.europa.eu/registration-dossier

[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] Urben, 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] U.S. EPA. ECOTOX Knowledgebase. Washington, DC: U.S. Environmental Protection Agency. URL: https://cfpub.epa.gov/ecotox/

[14] 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.

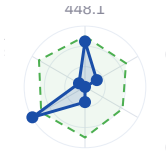
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External links

NIST: https://webbook.nist.gov/cgi/cbook.cgi?ID=121-54-0

ChEMBL: https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL221753

ADMET / Drug-likeness



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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