



SAFETY DATA SHEET

Cetyldimethylethylammonium bromide (Bretol)

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product name	Cetyldimethylethylammonium bromide (Bretol)
CAS number	124-03-8
EC number	204-672-8

1.2. Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Research and development.
Uses advised against	Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier	Molekula Ltd. Lingfield Way, Darlington, DL1 4XX, United Kingdom +44 (0) 3302000333 info@molekula.com
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1.4. Emergency telephone number

+44 (0) 7769276927

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (SI 2019 No. 720)

Physical hazards	Not Classified
Health hazards	Acute Tox. 4 - H302 Acute Tox. 4 - H332 Skin Irrit. 2 - H315 Eye Irrit. 2 - H319 STOT SE 3 - H335
Environmental hazards	Aquatic Acute 1 - H400 Aquatic Chronic 1 - H410

2.2. Label elements

EC number	204-672-8
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Hazard pictograms



Signal word	Warning
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Cetyldimethylethylammonium bromide (Bretol)

Hazard statements	H302+H332 Harmful if swallowed or if inhaled. H315 Causes skin irritation. H319 Causes serious eye irritation. H335 May cause respiratory irritation. H410 Very toxic to aquatic life with long lasting effects.
Precautionary statements	P261 Avoid breathing dust. P264 Wash contaminated skin thoroughly after handling. 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 CENTRE/doctor if you feel unwell. P302+P352 IF ON SKIN: Wash with plenty of water. 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. P330 Rinse mouth. P332+P313 If skin irritation occurs: Get medical advice/ attention. P337+P313 If eye irritation persists: Get medical advice/ attention. P362+P364 Take off contaminated clothing and wash it 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 in accordance with national regulations.

2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	Cetyldimethylethylammonium bromide (Bretol)
CAS number	124-03-8
EC number	204-672-8
Chemical formula	[CH ₃ (CH ₂) ₁₅ N(CH ₃) ₂ CH ₂ CH ₃]Br

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel.
Inhalation	Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Loosen tight clothing such as collar, tie or belt. Get medical attention if symptoms are severe or persist.
Ingestion	Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Never give anything by mouth to an unconscious person. Place unconscious person on their side in the recovery position and ensure breathing can take place. Keep affected person under observation. Get medical attention if symptoms are severe or persist.
Skin contact	Rinse with water.
Eye contact	Rinse with water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Get medical attention if any discomfort continues.

Cetyldimethylethylammonium bromide (Bretol)

Protection of first aiders First aid personnel should wear appropriate protective equipment during any rescue.

4.2. Most important symptoms and effects, both acute and delayed

General information The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation A single exposure may cause the following adverse effects: Temporary irritation.

Ingestion May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.

Skin contact Redness. Irritating to skin.

Eye contact Irritating to eyes.

4.3. Indication of any immediate medical attention and special treatment needed

Notes for the doctor Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media Combustible liquid. Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.

Unsuitable extinguishing media Do not use water jet as an extinguisher, as this will spread the fire.

5.2. Special hazards arising from the substance or mixture

Specific hazards This product is toxic.

Hazardous combustion products Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrous gases (NO_x). Hydrogen bromide (HBr).

5.3. Advice for firefighters

Protective actions during firefighting Avoid breathing fire gases or vapours. Evacuate area. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities.

Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment.

6.3. Methods and material for containment and cleaning up

Cetyldimethylethylammonium bromide (Bretol)

Methods for cleaning up

Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. Provide adequate ventilation. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions

Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

Advice on general occupational hygiene

Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions

Store away from incompatible materials (see Section 10). Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

Store at temperatures between 2°C/35.6°F and 8°C/46.4°F.

Storage class

Combustible solids that can not be assigned to any of the aforementioned LGK

7.3. Specific end use(s)

Specific end use(s)

The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure controls/Personal protection

8.1. Control parameters

Occupational exposure limits

STEL:

TWA:

8.2. Exposure controls

Protective equipment



Appropriate engineering controls

Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

Cetyldimethylethylammonium bromide (Bretol)

Hand protection	Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacture, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended.
Other skin and body protection	Wear appropriate clothing to prevent repeated or prolonged skin contact.
Hygiene measures	Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.
Respiratory protection	Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.
Environmental exposure controls	Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Appearance	Powder.
Colour	White.
Odour	Not known.
Odour threshold	No information available.
pH	No information available.
Melting point	No information available.
Initial boiling point and range	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Upper/lower flammability or explosive limits	No information available.
Vapour pressure	No information available.
Vapour density	No information available.
Relative density	No information available.
Solubility(ies)	No information available.
Partition coefficient	No information available.
Auto-ignition temperature	No information available.
Decomposition Temperature	No information available.

Cetyldimethylethylammonium bromide (Bretol)

9.2. Other information

Molecular weight 378.47

SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity See the other subsections of this section for further details.

10.2. Chemical stability

Stability Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions Violent reactions possible with: Strong oxidising agents.

10.4. Conditions to avoid

Conditions to avoid There are no known conditions that are likely to result in a hazardous situation.

10.5. Incompatible materials

Materials to avoid Avoid contact with strong oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Toxic gases or vapours.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Summary Harmful if swallowed.

Acute toxicity oral (LD₅₀ mg/kg) 500.0

Species Rat

ATE oral (mg/kg) 500.0

Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Summary Based on available data the classification criteria are not met.

ATE inhalation (dusts/mists mg/l) 1.5

Skin corrosion/irritation

Summary Causes skin irritation.

Serious eye damage/irritation

Summary Causes serious eye irritation.

Respiratory sensitisation

Summary Based on available data the classification criteria are not met.

Skin sensitisation

Cetyldimethylethylammonium bromide (Bretol)

Summary	Based on available data the classification criteria are not met.
<u>Germ cell mutagenicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Carcinogenicity</u>	
Summary	Based on available data the classification criteria are not met.
IARC carcinogenicity	None of the ingredients are listed or exempt.
<u>Reproductive toxicity</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - single exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Specific target organ toxicity - repeated exposure</u>	
Summary	Based on available data the classification criteria are not met.
<u>Aspiration hazard</u>	
Summary	Not relevant. Solid.
General information	The severity of the symptoms described will vary dependent on the concentration and the length of exposure.
Inhalation	A single exposure may cause the following adverse effects: Temporary irritation.
Ingestion	May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.
Skin contact	Redness. Irritating to skin.
Eye contact	Irritating to eyes.
Route of exposure	Ingestion Inhalation Skin and/or eye contact
Target organs	No specific target organs known.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity

Summary Very toxic to aquatic life.

LE(C)₅₀ $0.1 < L(E)C_{50} \leq 1$

M factor (Acute) 1

Chronic aquatic toxicity

Summary Very toxic to aquatic life with long lasting effects.

M factor (Chronic) 1

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient No information available.

12.4. Mobility in soil

Cetyldimethylethylammonium bromide (Bretol)

Mobility No data available.

12.5. Results of PBT and vPvB assessment

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous.

Disposal methods Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.

SECTION 14: Transport information

General For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section.

14.1. UN number

UN No. (ADR/RID) 3077

UN No. (IMDG) 3077

UN No. (ICAO) 3077

UN No. (ADN) 3077

14.2. UN proper shipping name

Proper shipping name (ADR/RID) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
(Cetyldimethylethylammonium bromide (Bretol))

Proper shipping name (IMDG) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
(Cetyldimethylethylammonium bromide (Bretol))

Proper shipping name (ICAO) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
(Cetyldimethylethylammonium bromide (Bretol))

Proper shipping name (ADN) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
(Cetyldimethylethylammonium bromide (Bretol))

14.3. Transport hazard class(es)

ADR/RID class 9

ADR/RID classification code M7

ADR/RID label 9

IMDG class 9

ICAO class/division 9

ADN class 9

Cetyldimethylethylammonium bromide (Bretol)

Transport labels



14.4. Packing group

ADR/RID packing group	III
IMDG packing group	III
ICAO packing group	III
ADN packing group	III

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant



14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

EmS	F-A, S-F
ADR transport category	3
Emergency Action Code	2Z
Hazard Identification Number (ADR/RID)	90
Tunnel restriction code	(-)

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
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15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

SECTION 16: Other information

Cetyldimethylethylammonium bromide (Bretol)

Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.
	ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.
	RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.
	IATA: International Air Transport Association.
	ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.
	IMDG: International Maritime Dangerous Goods.
	CAS: Chemical Abstracts Service.
	ATE: Acute Toxicity Estimate.
	LC50: Lethal Concentration to 50 % of a test population.
	LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).
	EC ₅₀ : 50% of maximal Effective Concentration.
	PBT: Persistent, Bioaccumulative and Toxic substance.
	vPvB: Very Persistent and Very Bioaccumulative.
Classification abbreviations and acronyms	Acute Tox. = Acute toxicity
	Eye Irrit. = Eye irritation
	Skin Irrit. = Skin irritation
	Aquatic Acute = Hazardous to the aquatic environment (acute)
	Aquatic Chronic = Hazardous to the aquatic environment (chronic)
Classification procedures according to SI 2019 No. 720	Acute Tox. 4 - H302: Skin Irrit. 2 - H315: Eye Irrit. 2 - H319: : Expert judgement. Aquatic Acute 1 - H400: Aquatic Chronic 1 - H410: : Expert judgement.
Training advice	Only trained personnel should use this material.
Revision date	06/01/2023
Revision	2
Supersedes date	15/12/2022
SDS number	1995
Hazard statements in full	H302 Harmful if swallowed.
	H315 Causes skin irritation.
	H319 Causes serious eye irritation.
	H332 Harmful if inhaled.
	H335 May cause respiratory irritation.
	H400 Very toxic to aquatic life.
	H410 Very toxic to aquatic life with long lasting effects.

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.