

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 26.02.2020

Version 6.8

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No.	818839
Product name	Tetra-n-butylammonium bromide for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	1643-19-2

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number **Please contact the regional company representation in your country.****SECTION 2. Hazards identification****2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

Acute toxicity, Category 4, Oral, H302

Eye irritation, Category 2, H319

Long-term (chronic) aquatic hazard, Category 3, H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Warning

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

CAS-No. 1643-19-2

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2)_4\text{NBr}$	$\text{C}_{16}\text{H}_{36}\text{BrN}$ (Hill)
EC-No.	216-699-2	
Molar mass	322,37 g/mol	

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Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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Tetrabutylammonium bromide ($\geq 80\%$ - $\leq 100\%$)

1643-19-2 *)

Acute toxicity, Category 4, H302

Eye irritation, Category 2, H319

Long-term (chronic) aquatic hazard, Category 3, H412

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

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hydrogen bromide, nitrogen oxides

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Protected from light.

Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	crystals
Colour	white
Odour	weakly amine-like
Odour Threshold	No information available.
pH	No information available.
Melting point	100 - 103 °C
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	No information available.
Relative vapour density	No information available.
Density	1,15 g/cm ³
Relative density	No information available.
Water solubility	600 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 1,71 (calculated) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.

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Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Bulk density	700 kg/m ³
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SECTION 10. Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD₅₀ Rat: > 300 - 2.000 mg/kg
OECD Test Guideline 423

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

LD₅₀ Rat: > 2.000 mg/kg
OECD Test Guideline 402

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Skin irritation

Rabbit

Result: slight irritation

OECD Test Guideline 404

Eye irritation

Rabbit

Result: Eye irritation

OECD Test Guideline 405

Causes serious eye irritation.

Sensitisation

Buehler Test Guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Mutagenicity (mammal cell test): chromosome aberration.

Human lymphocytes

Result: negative

Method: OECD Test Guideline 473

In vitro mammalian cell gene mutation test

Chinese hamster ovary cells

Result: negative

Method: OECD Test Guideline 476

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

After absorption:

We have no description of any symptoms of toxicity.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

static test LC50 Danio rerio (zebra fish): > 100 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 Daphnia magna (Water flea): 50 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

Toxicity to algae

static test ErC50 Chlorella vulgaris (Fresh water algae): 204,7 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

Toxicity to bacteria

EC50 Vibrio fischeri: 1,862 mg/l; 0,25 h
(ECHA)

12.2 Persistence and degradability

Biodegradability

0 %; 28 d; aerobic

(ECHA)

Not readily biodegradable.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,71

(calculated)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard Legislation	SEVESO III Not applicable
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Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 10 - 13

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H412	Harmful to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

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