

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 02.03.2018

Version 8.1

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

1.1 Product identifier

Catalogue No. 801603

Product name 1-Bromohexane 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. 111-25-1

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).

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603

Product name 1-Bromohexane for synthesis

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Flammable liquid, Category 3, H226

Skin irritation, Category 2, H315

Chronic aquatic toxicity, Category 2, H411

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H226 Flammable liquid and vapour.

H315 Causes skin irritation.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat.

P262 Do not get in eyes, on skin, or on clothing.

P273 Avoid release to the environment.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603
Product name 1-Bromohexane for synthesis

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

CAS-No. 111-25-1

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$\text{CH}_3(\text{CH}_2)_5\text{Br}$	$\text{C}_6\text{H}_{13}\text{Br}$ (Hill)
EC-No.	203-850-2	
Molar mass	165,07 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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1-Bromohexane ($\leq 100\%$)

111-25-1	*)	
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Flammable liquid, Category 3, H226

Skin irritation, Category 2, H315

Chronic aquatic toxicity, Category 2, H411

*) 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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

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. Remove contact lenses.

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed

The following applies to aliphatic halogenated hydrocarbons in general: systemic effect: narcosis, cardiovascular disorders. Toxic effect on liver, kidneys.
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.

Forms explosive mixtures with air at elevated temperatures.

Vapours are heavier than air and may spread along floors.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

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

Fire may cause evolution of:

hydrogen bromide

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

Remove container from danger zone and cool with water. 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: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

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.

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603
Product name 1-Bromohexane for synthesis

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:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 10 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 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (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

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	pleasant
Odour Threshold	No information available.
pH	No information available.
Melting point	-85 °C
Boiling point	No information available.
Flash point	47 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

Vapour pressure	4 hPa at 20 °C
Relative vapour density	No information available.
Density	1,18 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	< 1 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,8 (External MSDS) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The Safety Data Sheets for catalogue items are available at www.merckgroup.com

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
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The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents

10.4 Conditions to avoid

Heating.

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: > 2.000 mg/kg

OECD Test Guideline 401

Acute inhalation toxicity

LC50 Rat: 70 mg/l; 4 h ; vapour

(RTECS)

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: Irritations

(External MSDS)

Causes skin irritation.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603

Product name 1-Bromohexane for synthesis

Eye irritation

Rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

Maximisation Test Guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Result: negative

(own results)

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

The following applies to aliphatic halogenated hydrocarbons in general: systemic effect:

narcosis, cardiovascular disorders. Toxic effect on liver, kidneys.

Other dangerous properties can not be excluded.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 3,45 mg/l; 96 h
(External MSDS)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 Daphnia (water flea): 4,1 mg/l; 48 h
OECD Test Guideline 202

12.2 Persistence and degradability

Biodegradability

10 %; 28 d
OECD Test Guideline 301D
(External MSDS)
Not readily biodegradable.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 3,8

(External MSDS) 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

Additional ecological information

Discharge into the environment must be avoided.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
Product name	1-Bromohexane for synthesis

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 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (1-BROMOHEXANE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (1-BROMOHEXANE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	801603
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14.1 UN number	UN 1993
14.2 Proper shipping name	FLAMMABLE LIQUID, N.O.S. (1-BROMOHEXANE)
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
EmS	F-E S-E

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	SEVESO III
Legislation	FLAMMABLE LIQUIDS
	P5c
	Quantity 1: 5.000 t
	Quantity 2: 50.000 t
	SEVESO III
	ENVIRONMENTAL HAZARDS
	E2
	Quantity 1: 200 t
	Quantity 2: 500 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603
Product name 1-Bromohexane for synthesis

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

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 3

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.

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H411 Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 801603

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Signal word

Warning

Hazard statements

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H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat.

P273 Avoid release to the environment.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P313 Get medical advice/ attention.

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.