

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 26.05.2017

Version 11.12

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

1.1 Product identifier

Catalogue No. 803222

Product name Dibutylamine 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. 111-92-2

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).

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)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Flammable liquid, Category 3, H226
Acute toxicity, Category 4, Oral, H302
Acute toxicity, Category 2, Inhalation, H330
Acute toxicity, Category 3, Dermal, H311
Skin corrosion, Category 1A, H314

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

Danger

Hazard statements

H226 Flammable liquid and vapour.
H302 Harmful if swallowed.
H311 Toxic in contact with skin.
H314 Causes severe skin burns and eye damage.
H330 Fatal if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 803222
Product name Dibutylamine for synthesis

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H311 Toxic in contact with skin.

H314 Causes severe skin burns and eye damage.

H330 Fatal if inhaled.

Precautionary statements

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Contains: di-n-butylamine

Index-No. 612-049-00-0

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	(CH ₃ CH ₂ CH ₂ CH ₂) ₂ NH	C ₈ H ₁₉ N (Hill)
Index-No.	612-049-00-0	
EC-No.	203-921-8	

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Molar mass	129,24 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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di-n-butylamine ($\leq 100\%$)

111-92-2 *)

Flammable liquid, Category 3, H226

Acute toxicity, Category 4, H302

Acute toxicity, Category 2, H330

Acute toxicity, Category 3, H311

Skin corrosion, Category 1A, H314

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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

General advice

First aider needs to protect himself.

After inhalation: fresh air. Immediately call in physician.

If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

Headache, Nausea, Vomiting, conjunctivitis, Convulsions, CNS disorders, Unconsciousness
Irritation and corrosion, Cough, Shortness of breath
Risk of blindness!

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

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.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

Fire may cause evolution of:

Hydrogen cyanide (hydrocyanic acid), nitrous gases, 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

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

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

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.

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 803222
Product name Dibutylamine for synthesis

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. Keep locked up or in an area accessible only to qualified or authorised persons.

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.

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

Tightly fitting safety goggles

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 mm
Break through time:	> 30 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 730 Camatril® -Velours (full contact), KCL 720 Camapren® (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 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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Odour	amine-like
Odour Threshold	No information available.
pH	11,1 at 1 g/l 20 °C
Melting point	-62 °C
Boiling point/boiling range	160 °C at 1.013 hPa
Flash point	39 °C Method: c.c. DIN 51755 Part 1
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	0,6 %(V)
Upper explosion limit	6,8 %(V)
Vapour pressure	2,3 hPa at 20 °C
Relative vapour density	4,46
Density	0,76 g/cm ³ at 20 °C
Relative density	No information available.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Water solubility	3,8 g/l at 20 °C Method: OECD Test Guideline 105
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Partition coefficient: n-octanol/water	log Pow: 2,06 (experimental) Bioaccumulation is not expected.
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Auto-ignition temperature	No information available.
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Decomposition temperature	No information available.
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Viscosity, dynamic	0,9 mPa.s at 20 °C
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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9.2 Other data

Ignition temperature	260 °C DIN 51794
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SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitrosamines!

Exothermic reaction with:

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

acids, anhydrides, Strong oxidizing agents

Violent reactions possible with:

Alcohols, glycol ether, Ketones, Aldehydes, Esters, Nitriles, phenols

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

nonferrous metals, Light metals, Copper, Copper alloys, Tin

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: 550 mg/kg

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

absorption

Acute inhalation toxicity

LC50 Rat: 1,15 mg/l; 4 h ; vapour

OECD Test Guideline 403

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract, Inhalation may lead to the formation of oedemas in the respiratory tract.

absorption

Acute dermal toxicity

LD50 Rabbit: 770 mg/kg

absorption

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Skin irritation

Rabbit

Result: Causes severe burns.

Causes severe burns.

Eye irritation

Causes serious eye damage.

Risk of blindness!

conjunctivitis

Sensitisation

In animal experiments:

Result: negative

(IUCLID)

Germ cell mutagenicity

Genotoxicity in vivo

Mutagenicity (in vivo mammalian bone-marrow cytogenetic test, chromosomal analysis)

Mouse

male and female

Bone marrow

Result: negative

Method: OECD Test Guideline 475

Genotoxicity in vitro

Ames test

Result: negative

(IUCLID)

Mutagenicity (mammal cell test): chromosome aberration.

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

Application Route: Oral

Rat

Number of exposures: daily

Method: OECD Test Guideline 414

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

Systemic effects:

Headache, Nausea, Vomiting, CNS disorders, Convulsions, Unconsciousness

Damage to:

Kidney

Under given conditions, contact with nitrites or nitric acid can lead to the formation of nitrosamines, which have shown themselves to be carcinogenic in animal experiments.

This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 *Oncorhynchus mykiss* (rainbow trout): 5,5 mg/l; 96 h

(in soft water) (External MSDS)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

Toxicity to daphnia and other aquatic invertebrates

semi-static test LC50 Ceriodaphnia dubia (water flea): 8,4 mg/l; 48 h

Analytical monitoring: yes

Toxicity to algae

IC50 Desmodesmus subspicatus (green algae): 16,4 mg/l; 72 h
(IUCLID)

Toxicity to bacteria

EC50 Pseudomonas putida: 196 mg/l; 17 h
(IUCLID)

12.2 Persistence and degradability

Biodegradability

95 %; 28 d; aerobic

OECD Test Guideline 301C

Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,06

(experimental)

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine 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 2248
14.2 Proper shipping name	DI-N-BUTYLAMINE
14.3 Class	8 (3)
14.4 Packing group	II
14.5 Environmentally hazardous	--
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 2248
14.2 Proper shipping name	DI-N-BUTYLAMINE
14.3 Class	8 (3)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

14.1 UN number	UN 2248
14.2 Proper shipping name	DI-N-BUTYLAMINE
14.3 Class	8 (3)
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-E S-C
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	ACUTE TOXIC
	H2
	Quantity 1: 50 t
	Quantity 2: 200 t

	SEVESO III
	FLAMMABLE LIQUIDS
	P5c
	Quantity 1: 5.000 t
	Quantity 2: 50.000 t

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 803222
Product name Dibutylamine 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.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H330	Fatal if inhaled.

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.	803222
Product name	Dibutylamine for synthesis

Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.

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H330 Fatal if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat.

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Contains: di-n-butylamine

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	803222
Product name	Dibutylamine for synthesis

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.