

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 20.07.2015

Version 9.2

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

1.1 Product identifier

Catalogue No.	806917
Product name	Octylamine 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.	111-86-4

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

Identified uses	Chemical for synthesis Intermediate for use under strictly controlled conditions 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)

Flammable liquid, Category 3, H226
Corrosive to metals, Category 1, H290
Acute toxicity, Category 3, Oral, H301
Acute toxicity, Category 4, Inhalation, H332
Acute toxicity, Category 3, Dermal, H311
Skin corrosion, Category 1B, H314
Acute aquatic toxicity, Category 1, H400
Chronic aquatic toxicity, Category 1, H410

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

Classification (67/548/EEC or 1999/45/EC)

Xn	Harmful	R20/21/22
C	Corrosive	R34
N	Dangerous for the environment	R50/53

For the full text of the R-phrases 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
Danger

Hazard statements

H226 Flammable liquid and vapour.
H290 May be corrosive to metals.
H301 + H311 Toxic if swallowed or in contact with skin
H314 Causes severe skin burns and eye damage.
H332 Harmful if inhaled.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat.
P273 Avoid release to the environment.
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.
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.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word
Danger

Hazard statements

H301 + H311 Toxic if swallowed or in contact with skin
H314 Causes severe skin burns and eye damage.

Precautionary statements

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
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.

CAS-No. 111-86-4

2.3 Other hazards

None known.

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SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ (CH ₂) ₇ NH ₂	C ₈ H ₁₉ N (Hill)
EC-No.	203-916-0	
Molar mass	129,24 g/mol	

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

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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Octylamine (<= 100 %)

111-86-4 *)

Flammable liquid, Category 3, H226
Corrosive to metals, Category 1, H290
Acute toxicity, Category 3, H301
Acute toxicity, Category 4, H332
Acute toxicity, Category 3, H311
Skin corrosion, Category 1B, H314
Acute aquatic toxicity, Category 1, H400
Chronic aquatic toxicity, Category 1, H410

*) 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.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
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Octylamine (<= 100 %)

111-86-4 Xn, Harmful; R20/21/22
C, Corrosive; R34
N, Dangerous for the environment; R50/53

For the full text of the R-phrases 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. 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.

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If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Cough, Shortness of breath, Nausea, Vomiting, Dizziness, 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:

Ammonia, nitrogen oxides, nitrous gases

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

6.4 Reference to other sections

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Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

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

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. 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

The product is registered for use under strictly controlled conditions as defined in Article 18(4) of Regulation (EC) No. 1907/2006 (REACH) and must therefore be handled as such. Refer to the industry guidance prepared by Concawe, Cefic and EFCG for advice on the confirmation of strictly controlled conditions

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

splash contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm

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Break through time: > 120 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® (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
Odour	amine-like
Odour Threshold	No information available.
pH	No information available.
Melting point	-1 °C
Boiling point/boiling range	178 - 179 °C at 1.013 hPa Method: OECD Test Guideline 103
Flash point	60 °C Method: DIN 51755 Part 1
Evaporation rate	No information available.
Flammability (solid, gas)	Not applicable
Lower explosion limit	1,6 %(V)
Upper explosion limit	8,2 %(V)

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Vapour pressure	1 hPa at 20 °C
Relative vapour density	No information available.
Density	0,78 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,2 g/l at 25 °C
Partition coefficient: n-octanol/water	log Pow: 0,76 (External MSDS) Bioaccumulation is not expected.
Auto-ignition temperature	275 °C at 1.013 hPa Method: DIN 51794
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Ignition temperature	265 °C
Corrosion	May be corrosive to metals.

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability

Sensitive to air.

10.3 Possibility of hazardous reactions

Exothermic reaction with:

Acids

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

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Metals

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: < 200 mg/kg
OECD Test Guideline 401

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: 1,6 mg/l; 4 h ; dust/mist
OECD Test Guideline 403

Symptoms: Possible damages:, Cough, Shortness of breath, mucosal irritations, damage of respiratory tract, After a latency period:, Lung oedema
absorption

Acute dermal toxicity

LD50 Rabbit: 200 - 2.000 mg/kg
(ECHA)

absorption

Skin irritation

Rabbit

Result: Causes burns.

OECD Test Guideline 404

Causes burns.

Eye irritation

Risk of blindness!

Rabbit

Result: Causes serious eye damage.

OECD Test Guideline 405

Causes serious eye damage.

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vivo

Micronucleus test

Mouse

male

Oral

Bone marrow

Result: negative

Method: OECD Test Guideline 474

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Product name Octylamine for synthesis

Genotoxicity in vitro

reverse mutation assay

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

In vitro mammalian cell gene mutation test

Mouse lymphoma test

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.

Repeated dose toxicity

Rat

male and female

Oral

NOAEL: 100 mg/kg

OECD Test Guideline 422

Aspiration hazard

This information is not available.

11.2 Further information

After absorption:

Nausea, Vomiting, Dizziness, rise in blood pressure

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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

flow-through test LC50 Pimephales promelas (fathead minnow): 5,19 mg/l; 96 h

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 Daphnia magna (Water flea): 1,9 mg/l; 48 h

OECD Test Guideline 202

Toxicity to algae

static test EC50 Desmodesmus subspicatus (green algae): 0,23 mg/l; 72 h

Directive 67/548/EEC, Annex V, C.3.

static test NOEC Desmodesmus subspicatus (green algae): 0,01 mg/l; 72 h

Directive 67/548/EEC, Annex V, C.3.

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Toxicity to bacteria

static test NOEC activated sludge: ≥ 32 mg/l; 11 d

12.2 Persistence and degradability

Biodegradability

> 90 %; 28 d

OECD Test Guideline 301A

Readily biodegradable

> 60 %

OECD Test Guideline 302B

Moderately (partly) eliminable (DOC reduction 20-70 %).

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,76

(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

Discharge into the environment must be avoided.

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 2734

14.2 Proper shipping name AMINES, LIQUID, CORROSIVE, FLAMMABLE, N.O.S.
(OCTYLAMINE)

14.3 Class 8 (3)

14.4 Packing group I

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 2734

14.2 Proper shipping name AMINES, LIQUID, CORROSIVE, FLAMMABLE, N.O.S.
(OCTYLAMINE)

14.3 Class 8 (3)

14.4 Packing group I

14.5 Environmentally hazardous yes

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14.6 Special precautions for user no

Sea transport (IMDG)

14.1 UN number UN 2734

14.2 Proper shipping name AMINES, LIQUID, CORROSIVE, FLAMMABLE, N.O.S. (OCTYLAMINE)

14.3 Class 8 (3)

14.4 Packing group I

14.5 Environmentally hazardous yes

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	FLAMMABLE LIQUIDS P5c Quantity 1: 5.000 t Quantity 2: 50.000 t
	SEVESO III ENVIRONMENTAL HAZARDS E1 Quantity 1: 100 t Quantity 2: 200 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.

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

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals 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).

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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.
H290	May be corrosive to metals.
H301	Toxic if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H332	Harmful if inhaled.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

Full text of R-phrases referred to under sections 2 and 3

R20/21/22	Harmful by inhalation, in contact with skin and if swallowed.
R34	Causes burns.
R50/53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.
H290 May be corrosive to metals.
H301 + H311 Toxic if swallowed or in contact with skin
H314 Causes severe skin burns and eye damage.
H332 Harmful if inhaled.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response



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

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

Labelling (67/548/EEC or 1999/45/EC)

<i>Symbol(s)</i>	 C  N	Corrosive Dangerous for the environment
<i>R-phrases(s)</i>	20/21/22-34-50	Harmful by inhalation, in contact with skin and if swallowed. Causes burns. Very toxic to aquatic organisms.
<i>S-phrases(s)</i>	26-36/37/39-45-61	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Avoid release to the environment. Refer to special instructions/ Safety data sheets.

EC-No. 203-916-0

Reduced labelling (≤125 ml)

<i>Symbol(s)</i>	 C  N	Corrosive Dangerous for the environment
<i>R-phrases(s)</i>	20/21/22-34	Harmful by inhalation, in contact with skin and if swallowed. Causes burns.
<i>S-phrases(s)</i>	26-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

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.