

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 15.02.2019

Version 5.2

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

Catalogue No.	841022
Product name	n-Dodecyltrimethylammonium 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.	1119-94-4

**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 ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).
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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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

**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 3, Oral, H301  
Skin irritation, Category 2, H315  
Eye irritation, Category 2, H319  
Short-term (acute) aquatic hazard, Category 1, H400  
Long-term (chronic) aquatic hazard, Category 1, H410  
For the full text of the H-Statements mentioned in this Section, see Section 16.

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Product name

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n-Dodecyltrimethylammonium bromide for synthesis

## 2.2 Label elements

### Labelling (REGULATION (EC) No 1272/2008)

#### Hazard pictograms



Signal word  
Danger

#### Hazard statements

H301 Toxic if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H410 Very toxic to aquatic life with long lasting effects.

#### Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

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 ( $\leq 125$ ml)

##### Hazard pictograms



Signal word  
Danger

##### Hazard statements

H301 Toxic if swallowed.

##### Precautionary statements

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

CAS-No. 1119-94-4

## 2.3 Other hazards

None known.

## SECTION 3. Composition/information on ingredients

### 3.1 Substance

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Formula	C <sub>15</sub> H <sub>34</sub> BrN (Hill)
EC-No.	214-290-3
Molar mass	308,34 g/mol

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

*Chemical name (Concentration)*

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

1119-94-4   \*)

Acute toxicity, Category 3, H301  
Skin irritation, Category 2, H315  
Eye irritation, Category 2, H319  
Short-term (acute) aquatic hazard, Category 1, H400  
Long-term (chronic) aquatic hazard, Category 1, H410  
M-Factor: 10

\*) 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

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## SECTION 4. First aid measures

### 4.1 Description of first aid measures

*General advice*

First aider needs to protect himself.

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.

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

irritant effects, Cough, depressed respiration, Shortness of breath, agitation, spasms, cardiovascular disorders, CNS disorders

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Water, Foam, Carbon dioxide (CO<sub>2</sub>), 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:

hydrogen bromide, 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*

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

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## 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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

*Advice on safe handling*

Observe label precautions.

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## *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*

Tightly closed. Dry. Keep in a well-ventilated place. 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.

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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.

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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](http://www.kcl.de)).

*Other protective equipment*  
protective clothing

*Respiratory protection*

required when dusts are generated.

Recommended Filter type: Filter P 3 (acc. to DIN 3181) for solid and liquid particles of toxic and very toxic 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.

## 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	powder
Colour	white
Odour	odourless
Odour Threshold	Not applicable
pH	No information available.
Melting point	217 °C at 1.013,25 hPa Method: OECD Test Guideline 102 (decomposition)
Boiling point	No information available.
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	The product is not flammable. Test N.1: Test method for readily combustible solids
Lower explosion limit	No information available.
Upper explosion limit	No information available.

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Vapour pressure	< 1 hPa at 20 °C Method: OECD Test Guideline 104
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Relative vapour density	No information available.
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Density	1,17 g/cm <sup>3</sup> at 20 °C Method: OECD Test Guideline 109
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Relative density	No information available.
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Water solubility	> 954 g/l at 20 °C Method: OECD Test Guideline 105
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Partition coefficient: n-octanol/water	log Pow: -1,6 - -1,2 (20 °C) OECD Test Guideline 107 Bioaccumulation is not expected.
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Auto-ignition temperature	does not ignite
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Decomposition temperature	217 °C
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Viscosity, dynamic	No information available.
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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

Particle size	Mean particle size 29,6 µm Method: OECD Test Guideline 110
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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

sensitive to moisture

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

### 10.4 Conditions to avoid

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Moisture.

## 10.5 Incompatible materials

no information available

## 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: > 50 - 300 mg/kg

OECD Test Guideline 423

#### *Acute inhalation toxicity*

Symptoms: mucosal irritations, Cough, Shortness of breath

Symptoms: Possible damages:, damage of respiratory tract

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

In vitro study

Result: negative

OECD Test Guideline 431

In vitro study

Result: positive

OECD Test Guideline 439

Causes skin irritation.

#### *Eye irritation*

In vitro study

Result: positive

OECD Test Guideline 492

In vitro study

Result: positive

OECD Test Guideline 437

Causes serious eye irritation.

#### *Sensitisation*

Sensitisation test:

Result: negative

Method: OECD Test Guideline 442C

In vitro study

Result: negative

Method: OECD Test Guideline 442D

#### *Germ cell mutagenicity*



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## *Genotoxicity in vitro*

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

## *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**

Systemic effects:

If swallowed

CNS disorders, agitation, spasms, cardiovascular disorders, depressed respiration

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 daphnia and other aquatic invertebrates*

static test EC50 Daphnia magna (Water flea): 0,135 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

static test EC10 Daphnia magna (Water flea): 0,090 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

*Toxicity to algae*

static test ErC50 Desmodesmus subspicatus (green algae): 0,0599 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

static test EC10 Desmodesmus subspicatus (green algae): 0,00512 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

### **12.2 Persistence and degradability**

*Biodegradability*

73 %; 28 d; aerobic

OECD Test Guideline 301F

Readily biodegradable

### **12.3 Bioaccumulative potential**

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*Partition coefficient: n-octanol/water*

log Pow: -1,6 - -1,2 (20 °C)

OECD Test Guideline 107

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

*Surface tension*

39,3 mN/m

at 25 °C

Method: OECD Test Guideline 115

*Additional ecological information*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

**14.1 UN number** UN 2811

**14.2 Proper shipping name** TOXIC SOLID, ORGANIC, N.O.S. (N-DODECYLTRIMETHYLAMMONIUM BROMIDE)

**14.3 Class** 6.1

**14.4 Packing group** II

**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)

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<b>14.1 UN number</b>	UN 2811
<b>14.2 Proper shipping name</b>	TOXIC SOLID, ORGANIC, N.O.S. (N-DODECYLTRIMETHYLAMMONIUM BROMIDE)
<b>14.3 Class</b>	6.1
<b>14.4 Packing group</b>	II
<b>14.5 Environmentally hazardous</b>	yes
<b>14.6 Special precautions for user</b>	no

## Sea transport (IMDG)

<b>14.1 UN number</b>	UN 2811
<b>14.2 Proper shipping name</b>	TOXIC SOLID, ORGANIC, N.O.S. (N-DODECYLTRIMETHYLAMMONIUM BROMIDE)
<b>14.3 Class</b>	6.1
<b>14.4 Packing group</b>	II
<b>14.5 Environmentally hazardous</b>	yes
<b>14.6 Special precautions for user</b>	yes

EmS F-A S-A

**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 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 not regulated that deplete the ozone layer

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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

6.1B

## 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.

H301	Toxic if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H301 Toxic if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H410 Very toxic to aquatic life with long lasting effects.

*Precautionary statements*

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## Prevention

P273 Avoid release to the environment.

## Response

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.

## 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](http://www.wikipedia.org).

## Regional representation

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

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*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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