

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 8.4

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Denatonium Benzoate, United States  
Pharmacopeia (USP) Reference Standard

Product Number : 1171003  
Brand : US Pharmacopeia  
REACH No. : A registration number is not available for this substance as the  
substance or its uses are exempted from registration or the  
annual tonnage does not require a registration.  
CAS-No. : 3734-33-6

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Acute toxicity, (Category 4)	H302: Harmful if swallowed.
Acute toxicity, (Category 2)	H330: Fatal if inhaled.
Serious eye damage, (Category 1)	H318: Causes serious eye damage.

## 2.2 Label elements

### Labelling according Regulation (EC) No 1272/2008

#### Pictogram

Signal Word	Danger
Hazard Statements	
H302	Harmful if swallowed.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
Precautionary Statements	
P260	Do not breathe dust.
P264	Wash skin thoroughly after handling.
P280	Wear eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

### Reduced Labeling (<= 125 ml)

#### Pictogram

Signal Word	Danger
Hazard Statements	
H330	Fatal if inhaled.
H318	Causes serious eye damage.
Precautionary Statements	
P260	Do not breathe dust.
P280	Wear eye protection/ face protection.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

## 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

#### Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Formula : C<sub>21</sub>H<sub>29</sub>N<sub>2</sub>O · C<sub>7</sub>H<sub>5</sub>O<sub>2</sub>  
Molecular weight : 446,59 g/mol  
CAS-No. : 3734-33-6  
EC-No. : 223-095-2

Component		Classification	Concentration
<b>N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate</b>			
CAS-No.	3734-33-6	Acute Tox. 4; Acute Tox. 2; Eye Dam. 1; H302, H330, H318	<= 100 %
EC-No.	223-095-2		

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

### SECTION 4: First aid measures

#### 4.1 Description of first-aid measures

##### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

##### If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

##### In case of skin contact

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

##### In case of eye contact

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

##### If swallowed

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data 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**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

### **5.3 Advice 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.

### **5.4 Further information**

Suppress (knock down) gases/vapors/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 generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection 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**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

#### **Hygiene measures**

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

For precautions see section 2.2.

## **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 authorized persons.

### **Storage class**

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

## **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**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **Personal protective equipment**

##### **Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

##### **Skin protection**

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

##### **Full contact**

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

##### **Splash contact**

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

##### **Body Protection**

protective clothing

**Respiratory protection**

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P3

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.

**Control of environmental exposure**

Do not let product enter drains.

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**SECTION 9: Physical and chemical properties****9.1 Information on basic physical and chemical properties**

a) Physical state	crystalline
b) Color	white
c) Odor	odorless
d) Melting point/freezing point	Melting point/range: 163 - 171 °C at 960 hPa - OECD Test Guideline 102
e) Initial boiling point and boiling range	180 °C - OECD Test Guideline 103 - (decomposition)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	100 °C - closed cup - ISO 2719
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	6,5 - 7,5 at 30 g/l at 20 °C
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	45 g/l at 25 °C - (experimental)
n) Partition coefficient: n-octanol/water	log Pow: 2,06 at 25 °C - (ECHA)
o) Vapor pressure	No data available
p) Density	0,3846 g/cm <sup>3</sup> at 26 °C - OECD Test Guideline 109
Relative density	No data available

- |                             |                              |
|-----------------------------|------------------------------|
| q) Relative vapor density   | No data available            |
| r) Particle characteristics | No data available            |
|                             |                              |
| s) Explosive properties     | Not classified as explosive. |
| t) Oxidizing properties     | none                         |

## 9.2 Other safety information

Minimum ignition energy	2 - 4 mJ
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.  
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

No data available

### 10.4 Conditions to avoid

Avoid moisture.  
Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents

### 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 toxicity

LD50 Oral - Rat - 584 mg/kg

Remarks: (RTECS)

Oral: absorption

LD50 Oral - Rat - female - 648 mg/kg

Remarks: (ECHA)

Acute toxicity estimate Oral - 584 mg/kg

(ATE value derived from LD50/LC50 value)

LC50 Inhalation - Rat - male and female - 4 h - 0,2 mg/l - dust/mist

(OECD Test Guideline 403)

Remarks: (ECHA)

Acute toxicity estimate Inhalation - 0,2 mg/l - dust/mist

(ATE value derived from LD50/LC50 value)

LD50 Dermal - Rabbit - > 2.000 mg/kg

Remarks: (External MSDS)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation

Remarks: (ECHA)

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Corrosive

Remarks: (ECHA)

#### **Respiratory or skin sensitization**

Sensitisation test: - Guinea pig

Result: negative

Remarks: (External MSDS)

#### **Germ cell mutagenicity**

Test Type: Ames test

Metabolic activation: with and without metabolic activation

Method: US-EPA

Result: negative

Test Type: Mutagenicity (mammal cell test): micronucleus.

Method: OECD Test Guideline 474

Result: negative

#### **Carcinogenicity**

No data available

#### **Reproductive toxicity**

No data available

#### **Specific target organ toxicity - single exposure**

No data available

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

### **11.2 Additional Information**

#### **Endocrine disrupting properties**

##### **Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine



disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Systemic effects:

Drowsiness

Tremors

ataxia (impaired locomotor coordination)

Further data:

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 (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 500 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test EC50 - Chlorella vulgaris (Fresh water algae) - 281,556 mg/l - 72 h (OECD Test Guideline 201) Remarks: (ECHA)
Toxicity to bacteria	EC50 - Vibrio fischeri - 511,58 mg/l - 15 min Remarks: (ECHA)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 18,17 % - Not readily biodegradable. (OECD Test Guideline 301F)
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### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent,

bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

## 12.6 Endocrine disrupting properties

### **Product:**

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

## 12.7 Other adverse effects

Discharge into the environment must be avoided.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 2811

IMDG: 2811

IATA: 2811

### 14.2 UN proper shipping name

ADR/RID: TOXIC SOLID, ORGANIC, N.O.S. (N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate)

IMDG: TOXIC SOLID, ORGANIC, N.O.S. (N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate)

IATA: Toxic solid, organic, n.o.s. (N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate)

### 14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

### 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

### 14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

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## SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### National legislation

Seveso III: Directive 2012/18/EU of the H2 ACUTE TOXIC  
European Parliament and of the Council  
on the control of major-accident hazards  
involving dangerous substances.

#### Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

### 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

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## SECTION 16: Other information

### Full text of H-Statements

H302	Harmful if swallowed.
H318	Causes serious eye damage.
H330	Fatal if inhaled.

CHEMIKART

## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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