

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

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

Product Number : 1171003  
Brand : US Pharmacopeia  
CAS-No. : 3734-33-6

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week



## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

Acute toxicity (Oral) : Category 4

Acute toxicity (Inhalation) : Category 2

Serious eye damage : Category 1

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms : 

Signal word : Danger

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

Precautionary statements : **Prevention:**  
P260 Do not breathe dust.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P280 Wear eye protection/ face protection.  
P284 Wear respiratory protection.

#### **Response:**

P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.  
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.  
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

#### **Storage:**

P403 + P233 Store in a well-ventilated place. Keep



container tightly closed.  
P405 Store locked up.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 3734-33-6

**Components**

| Chemical name                                                                  | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|--------------------------------------------------------------------------------|-------------------|-----------------------|--------------|
| N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]-benzylammonium benzoate | 3734-33-6*        | $\geq 90 - \leq 100$  | -            |

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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### SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves. Show this 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.
- Most important symptoms and effects, : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in

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|                            |                                          |
|----------------------------|------------------------------------------|
| both acute and delayed     | section 11                               |
| Protection of first-aiders | : For personal protection see section 8. |
| Notes to physician         | : No data available                      |

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## SECTION 5. FIREFIGHTING MEASURES

|                                       |                                                                                |
|---------------------------------------|--------------------------------------------------------------------------------|
| Suitable extinguishing media          | : Water<br>Foam<br>Carbon dioxide (CO <sub>2</sub> )<br>Dry powder             |
| Unsuitable extinguishing media        | : For this substance/mixture no limitations of extinguishing agents are given. |
| Specific hazards during fire fighting | : Combustible.                                                                 |

Vapours 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.

|                               |                                                           |
|-------------------------------|-----------------------------------------------------------|
| Hazardous combustion products | : Carbon oxides<br><br>Nitrogen oxides (NO <sub>x</sub> ) |
|-------------------------------|-----------------------------------------------------------|

|                                |                     |
|--------------------------------|---------------------|
| Specific extinguishing methods | : No data available |
|--------------------------------|---------------------|

|                     |                                                                                                                                                                      |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Further information | : Suppress (knock down) gases/vapours/mists with a water spray jet.<br>Prevent fire extinguishing water from contaminating surface water or the ground water system. |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|

|                                        |                                                                                                            |
|----------------------------------------|------------------------------------------------------------------------------------------------------------|
| Special protective equipment for fire- | : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe |
|----------------------------------------|------------------------------------------------------------------------------------------------------------|



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**SECTION 6. ACCIDENTAL RELEASE MEASURES**

|                                                                     |                                                                                                                                                                                                                                                                                                                                 |
|---------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Personal precautions, protective equipment and emergency procedures | : Advice for non-emergency personnel:<br>Avoid generation and inhalation of dusts in all circumstances.<br>Avoid substance contact.<br>Ensure adequate ventilation.<br>Evacuate the danger area, observe emergency procedures, consult an expert.<br>Advice for emergency responders:<br>For personal protection see section 8. |
| Environmental precautions                                           | : Do not let product enter drains.                                                                                                                                                                                                                                                                                              |
| Methods and materials for containment and cleaning up               | : Cover drains. Collect, bind, and pump off spills.<br>Observe possible material restrictions (see sections 7 and 10).<br>Take up carefully. Dispose of properly. Clean up affected area.<br>Avoid generation of dusts.                                                                                                         |

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**SECTION 7. HANDLING AND STORAGE**

For precautions see section 2.2.

|                                           |                                                                                                                                                   |
|-------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| Advice on safe handling                   | : Work under hood. Do not inhale substance/mixture.                                                                                               |
| Further information on storage conditions | : Tightly closed.<br>Dry.<br>Keep in a well-ventilated place.<br>Keep locked up or in an area accessible only to qualified or authorised persons. |
| Storage class                             | : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials                                                                    |
| Recommended storage temperature           | : Recommended storage temperature see product label.                                                                                              |

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**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.



**Engineering measures** : No data available

### **Personal protective equipment**

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.

### **Hand protection**

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Full contact  
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.  
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)).

Eye 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 and body protection : protective clothing

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

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : crystalline

Color : white

Odor : odourless

Odor Threshold : No data available  
pH : 6.5 - 7.5 (68 °F / 20 °C)  
Concentration: 30 g/l

Melting point/ range : 325 - 340 °F / 163 - 171 °C  
(960 hPa)  
Method: OECD Test Guideline 102

Boiling point/boiling range : 356 °F / 180 °C  
Method: OECD Test Guideline 103  
(decomposition)

Flash point : 212 °F / 100 °C  
(968.9 hPa)  
Method: ISO 2719, closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /  
Upper flammability limit : No data available

Lower explosion limit /  
Lower flammability limit : No data available

Vapor pressure : No data available

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|                                        |                                                                               |
|----------------------------------------|-------------------------------------------------------------------------------|
| Relative vapour density                | : No data available                                                           |
| Relative density                       | : No data available                                                           |
| Density                                | : 0.3846 g/cm <sup>3</sup> (79 °F / 26 °C)<br>Method: OECD Test Guideline 109 |
| Solubility(ies)                        |                                                                               |
| Water solubility                       | : 45 g/l (experimental) (77 °F / 25 °C)                                       |
| Partition coefficient: n-octanol/water | : log Pow: 2.06 (77 °F / 25 °C)<br>Method: OECD Test Guideline 117 (ECHA)     |
| Autoignition temperature               | : No data available                                                           |
| Decomposition temperature              | : No data available                                                           |
| Viscosity, dynamic                     | : No data available                                                           |
| Viscosity, kinematic                   | : No data available                                                           |
| Flow time                              | : No data available                                                           |
| Explosive properties                   | : Not classified as explosive.                                                |
| Oxidizing properties                   | : none                                                                        |
| Molecular weight                       | : 446.59 g/mol                                                                |
| Minimum ignition energy                | : 2 - 4 mJ                                                                    |
| Particle characteristics               |                                                                               |
| Particle size                          | : No data available                                                           |

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## SECTION 10. STABILITY AND REACTIVITY

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.



|                                    |                                                                                           |
|------------------------------------|-------------------------------------------------------------------------------------------|
| Chemical stability                 | : The product is chemically stable under standard ambient conditions (room temperature) . |
| Possibility of hazardous reactions | : No data available                                                                       |
| Conditions to avoid                | : Avoid moisture.<br>Strong heating.                                                      |
| Incompatible materials             | : Strong oxidizing agents                                                                 |
| 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)

LC50 Inhalation - Rat - male and female - 4 h - 0.2 mg/l - dust/mist

(OECD Test Guideline 403)

Remarks: (ECHA)

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**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **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**

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

### Ecotoxicity

#### Components:

#### **N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate:**

|                                                     |                                                                                                                                                                      |
|-----------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | : LC50 (Danio rerio (zebra fish)): > 100 mg/l<br>Exposure time: 96 h<br>Test Type: static test<br>Method: OECD Test Guideline 203                                    |
| Toxicity to daphnia and other aquatic invertebrates | : EC50 (Daphnia magna (Water flea)): 500 mg/l<br>Exposure time: 48 h<br>Remarks: (ECHA)                                                                              |
| Toxicity to algae/aquatic plants                    | : EC50 (Chlorella vulgaris (Fresh water algae)): 281.556 mg/l<br>Exposure time: 72 h<br>Test Type: static test<br>Method: OECD Test Guideline 201<br>Remarks: (ECHA) |
| Toxicity to microorganisms                          | : EC50 (Vibrio fischeri): 511.58 mg/l<br>Exposure time: 15 min<br>Remarks: (ECHA)                                                                                    |

### Persistence and degradability

#### Components:

#### **N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate:**

|                  |                                                                                                                                                                  |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Biodegradability | : aerobic<br>Concentration: 100 mg/l<br>Result: Not readily biodegradable.<br>Biodegradation: 18.17 %<br>Exposure time: 28 d<br>Method: OECD Test Guideline 301F |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|

### Bioaccumulative potential

#### Components:

#### **N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate:**

|                                        |                                                                                       |
|----------------------------------------|---------------------------------------------------------------------------------------|
| Partition coefficient: n-octanol/water | : log Pow: 2.06 (77 °F / 25 °C)<br>Method: OECD Test Guideline 117<br>Remarks: (ECHA) |
|----------------------------------------|---------------------------------------------------------------------------------------|



**Mobility in soil**

No data available

**Other adverse effects****Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances  
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

**Components:****N,N-diethyl-N-[2-(2,6-dimethylphenylamino)-2-oxoethyl]- benzylammonium benzoate:**

Additional ecological information : Discharge into the environment must be avoided.

**Endocrine disrupting properties**

No data available

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**SECTION 13. DISPOSAL CONSIDERATIONS****Disposal methods**

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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**SECTION 14. TRANSPORT INFORMATION****International Regulations****IATA-DGR**

UN/ID No. : UN 2811  
Proper shipping name : Toxic solid, organic, n.o.s.  
(denatonium benzoate)  
Class : 6.1  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo aircraft) : 676  
Packing instruction (passenger aircraft) : 669

**IMDG-Code**

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UN number : UN 2811  
Proper shipping name : TOXIC SOLID, ORGANIC, N.O.S.  
(denatonium benzoate)  
Class : 6.1  
Packing group : II  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : no

### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National Regulations

#### 49 CFR

UN/ID/NA number : UN 2811  
Proper shipping name : Toxic solids, organic, n.o.s.  
(denatonium benzoate)  
Class : 6.1  
  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
ERG Code : 154  
Marine pollutant : no  
Poison Inhalation Hazard : No

### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.



### **Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

### **Clean Water Act**

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

#### **The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response;

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EHS - Extremely Hazardous Substance; 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; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation 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; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; 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

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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