

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Ethylbenzene

Product Number : 1265457
Brand : US Pharmacopeia
Index-No. : 601-023-00-4
CAS-No. : 100-41-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : 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.
SPRUCE ST 3050
63103 St. Louis

Telephone : (314) 771-5765
Telefax: (800) 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800 424 9300 (CHEMTREC) 24/7
+1 703 527 3887 (CHEMTREC) 24/7



SECTION 2. HAZARDS IDENTIFICATION

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

Hazards for the product as supplied

Flammable liquids	: Category 2
Acute toxicity (Inhalation)	: Category 4
Specific target organ toxicity - repeated exposure	: Category 2 (hearing organs)
Aspiration hazard	: Category 1
Short-term (acute) aquatic hazard	: Category 2
Long-term (chronic) aquatic hazard	: Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms	:	
Signal word	:	Danger
Hazard statements	:	H225 Highly flammable liquid and vapour. H304 May be fatal if swallowed and enters airways. H332 Harmful if inhaled. H373 May cause damage to organs (hearing organs) through prolonged or repeated exposure. H401 Toxic to aquatic life. H412 Harmful to aquatic life with long lasting effects.
Precautionary statements	:	Prevention: P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking. P233 Keep container tightly closed. P240 Ground/bond container and receiving equipment. P241 Use explosion-proof electrical/ ventilating/ lighting equipment. P242 Use only non-sparking tools.



P243 Take precautionary measures against static discharge.
P260 Do not breathe mist or vapours.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P314 Get medical advice/ attention if you feel unwell.
P331 Do NOT induce vomiting.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage:

P403 + P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Disposal:

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 100-41-4

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
ethylbenzene	100-41-4*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in

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If inhaled	: attendance. 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. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

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

Pay attention to flashback.

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



Forms explosive mixtures with air at ambient temperatures.

Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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: Wear appropriate personal protective equipment, as indicated in Section 8.
Environmental precautions	: Do not let product enter drains. Risk of explosion.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

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For precautions see section 2 GHS label elements

- Advice on protection against fire and explosion : Keep away from open flames, hot surfaces and sources of ignition.
Take precautionary measures against static discharge.
- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
Avoid generation of vapours/aerosols.
- Further information on storage conditions : Keep container tightly closed in a dry and well-ventilated place.
Keep away from heat and sources of ignition.
- Storage class : 3, Flammable liquids
- Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
ethylbenzene	100-41-4	TWA	100 ppm 435 mg/m ³	NIOSH REL
		ST	125 ppm 545 mg/m ³	NIOSH REL
		TWA	100 ppm 435 mg/m ³	OSHA Z-1

Biological occupational exposure limits

Components	CAS-No.	Control parameters	Biological specimen	Sampling time	Permissible concentration	Basis
ethylbenzene	100-41-4	Sum of mandelic acid and phenyl glyoxylic acid	Urine	End of shift (As soon as possible after exposure ceases)	150 mg/g creatinine	ACGIH BEI

Engineering measures : No data available



Personal protective equipment

Respiratory protection : required when vapours/aerosols 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 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.

Hand protection

Material : Viton®
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material : Nitrile rubber
Break through time : 10 min
Glove thickness : 0.4 mm
Protective index : Splash contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : 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).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : Flame retardant antistatic protective clothing.

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



with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Colour	: colourless
Odour	: aromatic
Odour Threshold	: No data available
pH	: No data available
Melting point/ range	: -138.8 °F / -94.9 °C (101.3 hPa) (ECHA)
Boiling point/boiling range	: 277.0 °F / 136.1 °C (1,013.3 hPa)
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: 806 °F / 430 °C 1,013 hPa
Upper explosion limit / Upper flammability limit	: Upper explosion limit 6.7 %(V)
Lower explosion limit / Lower flammability limit	: Lower explosion limit 1 %(V)
Vapour pressure	: 9.52 hPa (68 °F / 20 °C) Method: OECD Test Guideline 104
Relative vapour density	: No data available
Relative density	: 0.86 - 0.87 (68 °F / 20 °C)
Density	: 0.87 g/cm ³ (68 °F / 20 °C)

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Solubility(ies)	
Water solubility	: 0.2 g/l slightly soluble (77 °F / 25 °C) Method: Regulation (EC) No. 440/2008, Annex, A.6
Partition coefficient: n-octanol/water	: log Pow: 3.6 (68 °F / 20 °C) pH: 7.84 Method: Regulation (EC) No. 440/2008, Annex, A.8 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: 810 °F / 432 °C
Decomposition temperature	: No data available
Viscosity	
Viscosity, dynamic	: No data available
Viscosity, kinematic	: 0.773 mm ² /s (68 °F / 20 °C) Method: OECD Test Guideline 114 GLP: yes 0.641 mm ² /s (104 °F / 40 °C) Method: OECD Test Guideline 114 GLP: yes
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Surface tension	: 71.2 mN/m, 0.058 g/l, 73 °F / 23 °C, Surface tension, GLP: yes
Molecular weight	: 106.17 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapours may form explosive mixture with air.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous	: Violent reactions possible with:

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reactions	Strong oxidizing agents rubber various plastics
Conditions to avoid	: Warming.
Incompatible materials	: No data available
Hazardous decomposition products	: For Hazardous combustion products in the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 3,500 mg/kg

Remarks: (ECHA)

LC50 Inhalation - Rat - male - 4 h - 17.8 mg/l - vapour

Remarks: (ECHA)

LD50 Dermal - Rabbit - 15,433 mg/kg

Remarks: (RTECS)

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation - 24 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation

Remarks: (ECHA)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow



Application Route: Oral
Method: OECD Test Guideline 474
Result: negative

Test Type: unscheduled DNA synthesis assay
Species: Mouse

Application Route: Inhalation
Method: OECD Test Guideline 486
Result: negative

Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (ethylbenzene)
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

May cause damage to organs through prolonged or repeated exposure.

- hearing organs

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard

Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 d - No observed adverse effect level - 75 mg/kg

Central nervous system depression, Nausea, Headache, Vomiting, Ataxia., Tremors
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

CNS disorders
Tiredness
Drowsiness
Dizziness
Convulsions
Headache
narcosis

Handle in accordance with good industrial hygiene and safety practice.



SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

ethylbenzene:

Toxicity to fish	: LC50 (Oncorhynchus mykiss (rainbow trout)): 4.2 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 1.8 - 2.4 mg/l Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: US-EPA
Toxicity to algae/aquatic plants	: EC50 (Pseudokirchneriella subcapitata (green algae)): 3.6 mg/l Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: US-EPA GLP: yes
Toxicity to microorganisms	: EC50 (Photobacterium phosphoreum): 9.68 mg/l Exposure time: 30 min Remarks: (IUCLID)

Ecotoxicology Assessment

Acute aquatic toxicity : Toxic to aquatic life.

Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.

Persistence and degradability

Components:

ethylbenzene:

Biodegradability : aerobic



Inoculum: activated sludge
Concentration: 22 mg/l
Result: Readily biodegradable.
Biodegradation: ca. 79 %
Exposure time: 28 d
Method: ISO 14593
GLP: yes

Bioaccumulative potential

Components:

ethylbenzene:

Bioaccumulation : Remarks: Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

Partition coefficient: n-octanol/water : log Pow: 3.6 (68 °F / 20 °C)
pH: 7.84
Method: Regulation (EC) No. 440/2008, Annex, A.8
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

Components:

ethylbenzene:

Distribution among environmental compartments : Adsorption/Soil
Koc: 204, log Koc: 2.31
Method: (experimental)
Remarks: Moderately mobile in soils (Lit.)

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).

Endocrine disrupting properties

No data available



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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1175
Proper shipping name : Ethylbenzene
Class : 3
Packing group : II
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 364
Packing instruction (passenger aircraft) : 353

IMDG-Code

UN number : UN 1175
Proper shipping name : ETHYLBENZENE

Class : 3
Packing group : II
Labels : 3
EmS Code : F-E, S-D
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 1175
Proper shipping name : Ethylbenzene

Class : 3

Packing group : II
Labels : Class 3 - Flammable liquids
ERG Code : 130
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.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
ethylbenzene	100-41-4	1000	1000
ethylbenzene	100-41-4	100	100 (F003)

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 : Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

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). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

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).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489):

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

Clean Water Act

The following Hazardous Substances are listed under the U.S. CleanWater Act, Section 311, Table 116.4A:

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

The following Hazardous Chemicals are listed under the U.S. CleanWater Act, Section 311, Table 117.3:

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

This product contains the following toxic pollutants listed under the U.S. Clean Water Act Section 307

ethylbenzene 100-41-4 $\geq 90 - \leq 100 \%$

This product contains the following priority pollutants related to the U.S. Clean Water Act:



ethylbenzene

100-41-4

>= 90 - <= 100 %

US State Regulations**Massachusetts Right To Know**

ethylbenzene

100-41-4

Pennsylvania Right To Know

ethylbenzene

100-41-4

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

ethylbenzene

100-41-4

Washington Chemicals of High Concern

ethylbenzene

100-41-4

California Prop. 65

WARNING: This product can expose you to chemicals including ethylbenzene, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov. **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.

SECTION 16. OTHER INFORMATION
Full text of other abbreviations

ACGIH BEI : ACGIH - Biological Exposure Indices (BEI)
 NIOSH REL : USA. NIOSH Recommended Exposure Limits
 OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
 NIOSH REL / TWA : Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
 NIOSH REL / ST : STEL - 15-minute TWA exposure that should not be exceeded at any time during a workday
 OSHA Z-1 / TWA : 8-hour time weighted average

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; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response;

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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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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