

SAFETY DATA SHEET

Version 8.15 Revision Date 09/07/2024 Print Date 09/08/2024

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

1.1 Product identifiers

Product name : Ethylbenzene solution

Product Number : 487104 Brand : Aldrich

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

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-

527-3887 CHEMTREC (International) 24

Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302 Acute toxicity, Inhalation (Category 3), H331

Skin irritation (Category 2), H315 Eye irritation (Category 2A), H319 Carcinogenicity (Category 2), H351 Reproductive toxicity (Category 2), H361

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Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336 Specific target organ toxicity - repeated exposure, Oral (Category 1), Liver, Kidney, H372 Short-term (acute) aquatic hazard (Category 3), H402

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

2 GHS Label elements, including precautionary statements

Pictogram Signal Word Danger Hazard Statements Harmful if swallowed. H302 H315 Causes skin irritation. Causes serious eye irritation. H319 H331 Toxic if inhaled. May cause drowsiness or dizziness. H336 H351 Suspected of causing cancer. Suspected of damaging fertility or the unborn child. H361 Causes damage to organs (Liver, Kidney) through prolonged or H372 repeated exposure if swallowed. H402 Harmful to aquatic life. **Precautionary Statements** P201 Obtain special instructions before use. P202 Do not handle until all safety precautions have been read and understood. P260 Do not breathe mist or vapors. Wash skin thoroughly after handling. P264 P270 Do not eat, drink or smoke when using this product. P271 Use only outdoors or in a well-ventilated area. P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. P302 + P352 IF ON SKIN: Wash with plenty of soap and water. P304 + P340 + P311 IF INHALED: Remove person to fresh air and keep comfortable for breathing. 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 P308 + P313 IF exposed or concerned: Get medical advice/ attention. P332 + P313 If skin irritation occurs: Get medical advice/ attention. P337 + P313 If eye irritation persists: Get medical advice/ attention. P362 Take off contaminated clothing and wash before reuse. P403 + P233 Store in a well-ventilated place. Keep container tightly closed. P405 Store locked up. P501 Dispose of contents/ container to an approved waste disposal

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

plant.

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SECTION 3: Composition/information on ingredients

3.2 Mixtures

Component		Classification	Concentration		
Chloroform-D1-Deuteration					
CAS-No. EC-No. Registration	865-49-6 212-742-4	Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; Repr. 2;	>= 90 - <= 100 %		
number	01-2120242098-57- XXXX	STOT SE 3; STOT RE 1; Aquatic Acute 3; H302, H331, H315, H319, H351, H361, H336, H372, H402			
ethylbenzene					
CAS-No.	100-41-4	Flam. Liq. 2; Acute Tox. 4;	>= 0.1 - < 1		
EC-No.	202-849-4	STOT RE 2; Asp. Tox. 1;	%		
Index-No.	601-023-00-4	Aquatic Acute 2; Aquatic			
Registration number	01-2119489370-35- XXXX	Chronic 3; H225, H332, H373, H304, H401, H412			

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. 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: 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

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

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

Hydrogen chloride gas

Not combustible.

Ambient fire may liberate hazardous vapours.

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

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

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Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store under inert gas. Light sensitive. hygroscopic

Storage class

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Chloroform-D1- Deuteration	865-49-6	TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans		en with unknown relevance to
		ST	2 ppm 9.78 mg/m3	USA. NIOSH Recommended Exposure Limits

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		С	50 ppm 240 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	2 ppm 9.78 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
ethylbenzene	100-41-4	TWA	100 ppm 435 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	125 ppm 545 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	100 ppm 435 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	30 ppm 130 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	5 ppm 22 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

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Component	CAS-No.	Parameters	Value	Biological specimen	Basis
ethylbenzene	100-41-4	Sum of mandelic acid and phenyl glyoxylic acid	150mg/g creatinin e	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as	possible after exp	oosure ceases)

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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). Safety glasses

Skin protection

required

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter type AX



The entrepeneur 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.

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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

a)	Appearance	Form: liquid
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	рН	No data available
e)	Melting	No data available

Initial boiling point 60.9 °C 141.6 °F at 1,013 hPa and boiling range

g) Flash point ()No data available h) Evaporation rate No data available Flammability (solid, No data available gas)

Upper/lower j) flammability or explosive limits

point/freezing point

No data available

k) Vapor pressure No data available Vapor density No data available 1.500 g/cm3 m) Density

Relative density No data available n) Water solubility No data available o) Partition coefficient: No data available

n-octanol/water

p) Autoignition Not applicable temperature

q) Decomposition temperature

No data available

No data available Viscosity r)



s) Explosive properties Not classified as explosive.

t) Oxidizing properties none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

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

no information available

10.5 Incompatible materials

Bases, Strong oxidizing agents, Aluminum, Lithium, Sodium/sodium oxides, Magnesium

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Acute toxicity estimate Oral - 909 mg/kg

(Calculation method)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and

gastrointestinal tract.

Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

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Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Chloroform-D1-Deuteration)

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

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Chloroform-D1-

Deuteration)

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

Suspected of damaging the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

Mixture causes damage to organs through prolonged or repeated exposure.

- Liver, Kidney

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., Nausea, Dizziness, Headache Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components

Chloroform-D1-Deuteration

Acute toxicity

LD50 Oral - Rat - male - 908 mg/kg

(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: Chloroform

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor

(Expert judgment)

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

3.1/3.2)

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The value is given in analogy to the following substances: Chloroform

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (ECHA)

The value is given in analogy to the following substances: Chloroform Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.

Remarks: (ECHA)

The value is given in analogy to the following substances: Chloroform

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.6)

Remarks: The value is given in analogy to the following substances: Chloroform

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative Remarks: (ECHA)

The value is given in analogy to the following substances: Chloroform

Test Type: unscheduled DNA synthesis assay

Test system: Liver Result: negative Remarks: (ECHA)

The value is given in analogy to the following substances: Chloroform

Method: OECD Test Guideline 474

Species: Rat - male and female - Red blood cells (erythrocytes)

Result: negative

Remarks: The value is given in analogy to the following substances: Chloroform

Method: OECD Test Guideline 486 Species: Rat - male - Liver cells

Result: negative

Remarks: The value is given in analogy to the following substances: Chloroform

Species: Mouse - female

Result: negative Remarks: (ECHA)

The value is given in analogy to the following substances: Chloroform

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

Suspected of damaging the unborn child.

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

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Remarks: The value is given in analogy to the following substances: Chloroform

Specific target organ toxicity - repeated exposure

Oral - Causes damage to organs through prolonged or repeated exposure.

- Liver, Kidney

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

3.1/3.2)

The value is given in analogy to the following substances: Chloroform

Aspiration hazard

No data available

ethylbenzene

Acute toxicity

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

Remarks: (ECHA)

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

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

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Method: OECD Test Guideline 474 Species: Mouse - male - Bone marrow

Result: negative

Method: OECD Test Guideline 486 Species: Mouse - male and female

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

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 edema and pneumonitis.

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

Chloroform-D1-Deuteration

Toxicity to algae static test ErC50 - Chlamydomonas reinhardtii (green algae) -

13.3 mg/l - 72 h Remarks: (ECHA)

The value is given in analogy to the following substances:

Chloroform

Toxicity to bacteria Remarks: (ECHA)

The value is given in analogy to the following substances:

Chloroform

Toxicity to daphnia semi-static test NOEC - Daphnia magna (Water flea) - 6.3 mg/l

and other aquatic - 21 d

invertebrates(Chronic Remarks: (ECHA)

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The value is given in analogy to the following substances: toxicity)

The value is given in analogy to the following substances:

Chloroform

ethylbenzene

Toxicity to fish semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) -

4.2 mg/l - 96 h

(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic

static test EC50 - Daphnia magna (Water flea) - 1.8 - 2.4 mg/l

invertebrates

- 48 h (US-EPA)

Toxicity to algae static test EC50 - Pseudokirchneriella subcapitata (green algae)

- 3.6 mg/l - 96 h

(US-EPA)

EC50 - Photobacterium phosphoreum - 9.68 mg/l - 30 min Toxicity to bacteria

Remarks: (IUCLID)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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

DOT (US)

UN number: 1888 Class: 6.1 Packing group: III

Proper shipping name: ChloroformSOLUTION

Reportable Quantity (RQ): 10 lbs Reportable Quantity (RQ): 10 lbs Reportable Quantity (RQ): 100 lbs Poison Inhalation Hazard: No

IMDG

UN number: 1888 Class: 6.1 Packing group: III EMS-No: F-A, S-A

Proper shipping name: CHLOROFORMSOLUTION

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IATA

UN number: 1888 Class: 6.1 Packing group: III

Proper shipping name: ChloroformSOLUTION

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Chloroform-D1-Deuteration	865-49-6	10	10
Chloroform-D1-Deuteration	865-49-6	10	10 (D022)
ethylbenzene	100-41-4	100	100 (F003)

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Chloroform-D1-Deuteration	865-49-6	10	10

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
Chloroform-D1-Deuteration	865-49-6	10000

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

SARA 313 : The following components are subject to reporting

levels established by SARA Title III, Section 313:

Chloroform- 865-49-6 >= 90 - <= 100 %

D1-Deuteration

ethylbenzene 100-41-4 >= 0.1 - < 1 %

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):

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

The following chemical(s) are listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F):

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

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

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

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Clean Water Act

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

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

ethylbenzene 100-41-4 >= 0.1 - < 1 %

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

Table 117.3:

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

ethylbenzene 100-41-4 >= 0.1 - < 1 %

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

Section 307

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

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

Chloroform-D1- 865-49-6 >= 90 - <= 100 %

Deuteration

US State Regulations

Massachusetts Right To Know

Chloroform-D1-Deuteration 865-49-6

Pennsylvania Right To Know

Chloroform-D1-Deuteration 865-49-6 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 Chloroform-D1-Deuteration, ethylbenzene, which is/are known to the State of California to cause cancer, and Chloroform-D1-Deuteration, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on 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

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

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