

# SAFETY DATA SHEET

Version 8.8  
Revision Date 07/14/2021  
Print Date 10/25/2021

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

### 1.1 Product identifiers

Product name : Ethylbenzene solution

Product Number : 736198  
Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

### 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)

Flammable liquids (Category 4), H227  
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  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336  
Specific target organ toxicity - repeated exposure, Oral (Category 1), Liver, Kidney, H372  
Specific target organ toxicity - repeated exposure (Category 2), hearing organs, H373  
Short-term (acute) aquatic hazard (Category 3), H402

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

### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H227 Combustible liquid.  
H302 Harmful if swallowed.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H331 Toxic if inhaled.  
H336 May cause drowsiness or dizziness.  
H351 Suspected of causing cancer.  
H361 Suspected of damaging fertility or the unborn child.  
H372 Causes damage to organs (Liver, Kidney) through prolonged or repeated exposure if swallowed.  
H373 May cause damage to organs (hearing organs) through prolonged or repeated exposure.  
H402 Harmful to aquatic life.

Precautionary statement(s)

P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.  
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.  
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 rinsing.  
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.  
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.  
P405 Store locked up.  
P501 Dispose of contents/ container to an approved waste disposal plant.

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

## SECTION 3: Composition/information on ingredients

### 3.2 Mixtures

Formula : C<sub>8</sub>H<sub>10</sub>  
Molecular weight : 120.39 g/mol

Component		Classification	Concentration
<b>Chloroform-D1-Deuteration</b>			
CAS-No.	865-49-6	Acute Tox. 4; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; Carc. 2; Repr. 2; STOT SE 3; STOT RE 1; Aquatic Acute 3; H302, H331, H315, H319, H351, H361, H336, H372, H402 Concentration limits: 20 %: STOT SE 3, H336;	>= 90 - <= 100 %
EC-No.	212-742-4		
Registration number	01-2120242098-57-XXXX		
<b>ethylbenzene</b>			
CAS-No.	100-41-4	Flam. Liq. 2; Acute Tox. 4; Carc. 2; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H332, H351, H373, H304, H401, H412	>= 5 - < 10 %
EC-No.	202-849-4		
Index-No.	601-023-00-4		

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**

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

Hydrogen chloride gas

Mixture with combustible ingredients.

Vapors are heavier than air and may spread along floors.

Risk of dust explosion.

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**

Remove container from danger zone and cool with water. 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: Do not breathe vapors, 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.

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.

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

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

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

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

### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

### 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.

### Storage stability

Recommended storage temperature

15 - 25 °C

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

## 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

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		
		ST	2 ppm 9.78 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		

		C	50 ppm 240 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	2 ppm 9.78 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	2 ppm 9.78 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
ethylbenzene	100-41-4	TWA	100 ppm 435 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	30 ppm 130 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	5 ppm 22 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
ethylbenzene	100-41-4	Sum of mandelic acid and phenyl glyoxylic acid	0.15g/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure 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

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.

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### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: liquid   |
| b) Odor   | No data available  |
| c) Odor Threshold                               | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | -64 °C (-83 °F)  |
| f) Initial boiling point and boiling range      | 60.90 °C 141.62 °F at 1,013 hPa  |
| g) Flash point                                  | > 60 °C (> 140 °F) at ca.1,019.2 hPa - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 - Not classified due to data which are conclusive although insufficient for classification. |
| h) Evaporation rate                             | No data available  |
| i) Flammability (solid, gas)                    | No data available  |
| j) Upper/lower flammability or explosive limits | No data available  |
| k) Vapor pressure                               | No data available  |
| l) Vapor density                                | No data available  |
| m) Density                                      | 1.5000 g/cm <sup>3</sup>   |
| Relative density                                | No data available  |
| n) Water solubility                             | No data available  |
| o) Partition coefficient: n-octanol/water       | No data available  |
| p) Autoignition temperature                     | No data available  |
| q) Decomposition temperature                    | No data available  |
| r) Viscosity                                    | No data available  |
| s) Explosive properties                         | No data available  |
| t) Oxidizing properties                         | No data available  |

#### 9.2 Other safety information

No data available

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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.

### 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

Strong heating.

### 10.5 Incompatible materials

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

### 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

#### Mixture

#### Acute toxicity

Acute toxicity estimate Oral - 950.22 mg/kg  
(Calculation method)

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

Acute toxicity estimate Inhalation - 4 h - 3.26 mg/l  
(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

#### Skin corrosion/irritation

Mixture causes skin irritation.

#### Serious eye damage/eye irritation

Mixture causes serious eye irritation.

#### 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: No ingredient 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**

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

Mixture may cause damage to organs through prolonged or repeated exposure. - hearing organs

**Aspiration hazard**

No data available

**11.2 Additional Information**

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)

Inhalation: No data available

Dermal: No data available

**Skin corrosion/irritation**

Skin - Rabbit

Result: Irritating to skin. - 24 h

Remarks: (ECHA)

Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Irritating to eyes.

Remarks: (ECHA)

**Respiratory or skin sensitization**

Maximization Test - Guinea pig

Result: negative

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

**Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test  
Test system: mouse lymphoma cells  
Result: positive  
Remarks: (ECHA)  
Species: Rat - male - Bone marrow  
Result: positive  
Remarks: (ECHA)

**Carcinogenicity**

Suspected of causing cancer.

**Reproductive toxicity**

Suspected of damaging the unborn child.

**Specific target organ toxicity - single exposure**

May cause drowsiness or dizziness.

Remarks: (in analogy to similar products)

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)

**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

Remarks: (ECHA)

LD50 Dermal - Rabbit - 15,433 mg/kg

Remarks: (RTECS)

No data available

**Skin corrosion/irritation**

Skin - Rabbit

Result: Moderate skin irritation - 24 h

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Mild eye irritation

Remarks: (ECHA)

**Respiratory or skin sensitization**

Patch test: - Human

Result: negative

Remarks: (IUCLID)

**Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test):

Test system: Mouse lymphoma test

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: Hamster

Test system: ovary

Result: negative

Method: OECD Test Guideline 474

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

**Aspiration hazard**

May be fatal if swallowed and enters airways.

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**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 Other adverse effects**

No data available

**Components****Chloroform-D1-Deuteration**

Toxicity to daphnia  
and other aquatic  
invertebrates

static test EC50 - Daphnia magna (Water flea) - 79 mg/l - 48 h  
Remarks: (ECHA)

Toxicity to algae static test ErC50 - Chlamydomonas reinhardtii (green algae) - 13.3 mg/l - 72 h  
Remarks: (ECHA)

Toxicity to bacteria static test EC50 - activated sludge - 0.48 mg/l - 24 h  
Remarks: (ECHA)

### **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 invertebrates static test EC50 - Daphnia magna (Water flea) - 1.8 - 2.4 mg/l - 48 h  
(US-EPA)

Toxicity to algae static test EC50 - Pseudokirchneriella subcapitata (green algae) - 3.6 mg/l - 96 h  
(US-EPA)

Toxicity to bacteria EC50 - Photobacterium phosphoreum - 9.68 mg/l - 30 min  
Remarks: (IUCLID)

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

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## **SECTION 14: Transport information**

### **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  
Poison Inhalation Hazard: No

### **IMDG**

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

### **IATA**

UN number: 1888 Class: 6.1 Packing group: III

Proper shipping name: ChloroformSOLUTION

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**SECTION 15: Regulatory information****SARA 302 Components**

Chloroform-D1-Deuteration	CAS-No. 865-49-6	Revision Date 2008-11-03
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**SARA 313 Components**

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

Chloroform-D1-Deuteration	CAS-No. 865-49-6	Revision Date 2008-11-03
ethylbenzene	100-41-4	2007-07-01

**Reportable Quantity** : D022 lbs

**Massachusetts Right To Know Components**

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

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**SECTION 16: Other information****Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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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