SAFETY DATA SHEET

Version 8.12
Revision Date 03/01/2024
Print Date 06/20/2024

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

1.1 Product identifiers

Product name : Ethylbenzene solution

Product Number : 612065
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)

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
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 Statements

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.
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.
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.
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 plant.

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Molecular weight : 120.39 g/mol

Component		Classification	Concentration
Chloroform-D1-Deuteration			
CAS-No. EC-No. Registration number	865-49-6 212-742-4 01-2120242098-57-XXXX	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	>= 90 - <= 100 %
ethylbenzene			
CAS-No. EC-No. Index-No. Registration number	100-41-4 202-849-4 601-023-00-4 01-2119489370-35-XXXX	Flam. Liq. 2; Acute Tox. 4; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H332, H373, H304, H401, H412	>= 0.1 - < 1 %

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

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.

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		
		ST	2 ppm 9.78 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential Occupational Carcinogen		

		C	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

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
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

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: clear, liquid Color: colorless
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -64 °C (-83 °F)
f)	Initial boiling point and boiling range	60.9 °C 141.6 °F at 1,013 hPa
g)	Flash point	()No data available
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	1.500 g/cm3
	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	Not applicable
q)	Decomposition temperature	No data available

r)	Viscosity	No data available
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 - 908 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.

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

Vomiting, Gastrointestinal disturbance, Exposure to and/or consumption of alcohol may increase toxic effects., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
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)
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.
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 and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 6.3 mg/l - 21 d Remarks: (ECHA) The value is given in analogy to the following substances: 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 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)

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

IATA
UN number: 1888 Class: 6.1 Packing group: III
Proper shipping name: ChloroformSOLUTION

SECTION 15: Regulatory information

SARA 302 Components

	CAS-No.	Revision Date
Chloroform-D1-Deuteration	865-49-6	2008-11-03

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

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

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

Reportable Quantity : D022 lbs

F003 lbs

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Chloroform-D1-Deuteration	865-49-6	2008-11-03

Pennsylvania Right To Know Components

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

California Prop. 65 Components

	CAS-No.	Revision Date
, which is/are known to the State of California to cause cancer, andChloroform-D1-Deuteration	865-49-6	2011-09-01

ethylbenzene	100-41-4	2007-09-28

, 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.Chloroform-D1-Deuteration	CAS-No. 865-49-6	Revision Date 2011-09-01

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.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

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