

## SAFETY DATA SHEET

Version 5.6  
Revision Date 09/23/2016  
Print Date 10/20/2019

---

1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Ethyl-1,1-d<sub>2</sub> benzene-d<sub>5</sub>

Product Number : 587060  
Brand : Aldrich  
Index-No. : 601-023-00-4

CAS-No. : 84272-90-2

## 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

---

2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

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

Flammable liquids (Category 2), H225  
Acute toxicity, Inhalation (Category 4), H332  
Carcinogenicity (Category 2), H351

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)

H225 : Highly flammable liquid and vapour.  
H332 : Harmful if inhaled.  
H351 : Suspected of causing cancer.

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.  
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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
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.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Chemical characterization	: Isotopically labeled
Formula	: C <sub>8</sub> D <sub>7</sub> H <sub>3</sub>
Molecular weight	: 113.21 g/mol
CAS-No.	: 84272-90-2
Index-No.	: 601-023-00-4

#### Hazardous components

Component	Classification	Concentration
<b>Ethyl-1,1-d2 benzene-d5</b>		
	Flam. Liq. 2; Acute Tox. 4; Carc. 2; H225, H332, H351	<= 100 %

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

---

## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

---

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 6.4 Reference to other sections

For disposal see section 13.

---

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

### 7.3 Specific end use(s)

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

---

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Ethyl-1,1-d2 benzene-d5	84272-90-2	TWA	20.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Cochlear impair Kidney damage (nephropathy) Upper Respiratory Tract irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans		

		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Cochlear impair Kidney damage (nephropathy) Upper Respiratory Tract irritation Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans		
		STEL	125.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Central Nervous System impairment Upper Respiratory Tract irritation Eye irritation Adopted values or notations enclosed are those for which changes are proposed in the NIC See Notice of Intended Changes (NIC) Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans		
		TWA	100.000000 ppm 435.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		TWA	100.000000 ppm 435.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	125.000000 ppm 545.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	5 ppm 22 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	30 ppm 130 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
Ethyl-1,1-d2 benzene-d5	84272-90-2	Sum of mandelic acid and phenyl glyoxylic acid	0.7g/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			
		Ethylbenzene		In end-exhaled air	ACGIH - Biological Exposure Indices (BEI)
		Not critical			
		Sum of mandelic acid and phenyl glyoxylic acid	0.15g/g creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Colour: colourless
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -95 °C (-139 °F)
f) Initial boiling point and boiling range	136 °C (277 °F) - lit.
g) Flash point	22 °C (72 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	0.923 g/mL at 25 °C (77 °F) 0.923 g/cm <sup>3</sup> at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition 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

---

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

---

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

#### Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Ethyl-1,1-d2 benzene-d5)

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 identified as a carcinogen or potential carcinogen by OSHA.

#### Reproductive toxicity

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

Central nervous system depression, Nausea, Headache, Vomiting, Ataxia., Tremors

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

---

**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

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

---

**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

---

**14. TRANSPORT INFORMATION****DOT (US)**

UN number: 1175      Class: 3  
Proper shipping name: Ethylbenzene  
Reportable Quantity (RQ): 1000 lbs

Packing group: II

Poison Inhalation Hazard: No

**IMDG**

UN number: 1175      Class: 3  
Proper shipping name: ETHYLBENZENE

Packing group: II

EMS-No: F-E, S-D

**IATA**

UN number: 1175      Class: 3  
Proper shipping name: Ethylbenzene

Packing group: II

---

**15. REGULATORY INFORMATION****SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

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

#### **SARA 311/312 Hazards**

Fire Hazard, Chronic Health Hazard

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

	CAS-No.	Revision Date
Ethyl-1,1-d2 benzene-d5	84272-90-2	2009-07-17

#### **Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Ethyl-1,1-d2 benzene-d5	84272-90-2	2009-07-17

#### **New Jersey Right To Know Components**

	CAS-No.	Revision Date
Ethyl-1,1-d2 benzene-d5	84272-90-2	2009-07-17

#### **California Prop. 65 Components**

WARNING! This product contains a chemical known to the State of California to cause cancer.

	CAS-No.	Revision Date
Ethyl-1,1-d2 benzene-d5	84272-90-2	2007-09-28

---

## **16. OTHER INFORMATION**

#### **Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
Carc.	Carcinogenicity
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H332	Harmful if inhaled.
H351	Suspected of causing cancer.

#### **HMIS Rating**

Health hazard:	1
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

#### **NFPA Rating**

Health hazard:	1
Fire Hazard:	3
Reactivity Hazard:	0

#### **Further information**

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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.

#### **Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 5.6

Revision Date: 09/23/2016

Print Date: 10/20/2019