

SAFETY DATA SHEET

Version 8.3
Revision Date 07.09.2021
Print Date 29.04.2023

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

1.1 Product identifiers

Product name : Ethylbenzene for synthesis
Product Number : 8.01372
Catalogue No. : 801372
Brand : Millipore
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 : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

Company : SIGMA-ALDRICH CANADA LTD.
2149 WINSTON PARK DRIVE
OAKVILLE ON L6H 6J8
CANADA
Telephone : +1 905 829-9500
Fax : +1 905 829-9292

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 Hazardous Products Regulations (HPR) (SOR/2015-17)

Flammable liquids (Category 2), H225
Acute toxicity, Inhalation (Category 4), H332
Specific target organ toxicity - repeated exposure (Category 2), hearing organs, H373
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 3), H412

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 vapor.
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 statement(s)

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
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 + 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.
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.
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

3.1 Substances

Formula : C₈H₁₀
Molecular weight : 106.17 g/mol
CAS-No. : 100-41-4
EC-No. : 202-849-4
Index-No. : 601-023-00-4

Component	Classification	Concentration *
ethylbenzene		
	Flam. Liq. 2; Acute Tox. 4; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 3; H225, H332, H373, H304, H401, H412	<= 100 %
* Weight %		

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

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.

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

Water Carbon dioxide (CO₂) Foam 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

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

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

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Forms explosive mixtures with air at ambient temperatures.

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. 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. 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. Risk of explosion.

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.

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
ethylbenzene	100-41-4	STEL	125 ppm 543 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
		TWA	100 ppm 434 mg/m ³	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
		TWA	20 ppm	Canada. British Columbia OEL
Remarks	IARC '2B' applies to substances deemed possibly carcinogenic to humans.			
		TWAEV	20 ppm	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
	Carcinogenic effect detected in animals. Results of studies relating to the carcinogenicity of these substances in animals are not necessarily applicable to humans.			

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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 EN374 please

contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 10 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

Flame retardant antistatic 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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|--|
| a) Appearance | Form: liquid
Color: colorless |
| b) Odor | aromatic |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | -94.9 °C (-138.8 °F) at 101.3 hPa - (ECHA) |
| f) Initial boiling point and boiling range | 136.1 °C 277.0 °F at 1,013.3 hPa |
| g) Flash point | 23 °C (73 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 6.7 %(V)
Lower explosion limit: 1 %(V) |
| k) Vapor pressure | 9.52 hPa at 20 °C (68 °F) - OECD Test Guideline 104 |
| l) Vapor density | No data available |
| m) Density | 0.87 g/cm ³ at 20 °C (68 °F) |
| Relative density | 0.86 - 0.87 at 20 °C (68 °F) |
| n) Water solubility | 0.2 g/l at 25 °C (77 °F) - Regulation (EC) No. 440/2008, Annex, A.6 - slightly soluble |
| o) Partition coefficient: n-octanol/water | Pow: 4,170; log Pow: 3.6 at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.8 |

- p) Autoignition temperature 430 °C (806 °F) at 1,013 hPa
- q) Decomposition temperature No data available
- r) Viscosity 0.773 mm²/s at 20 °C (68 °F) - OECD Test Guideline 114 -
- s) Explosive properties No data available
- t) Oxidizing properties none

9.2 Other safety information

Surface tension 71.2 mN/m at 23 °C (73 °F)

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition 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

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)

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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

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Hamster

Test system: ovary

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: Mutagenicity (in vivo mammalian bone-marrow cytogenetic test, chromosomal analysis)

Species: Mouse

Application Route: Inhalation

Method: OECD Test Guideline 474

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.

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 90 d - NOAEL (No observed adverse effect level) - 75 mg/kg - LOAEL (Lowest observed adverse effect level) - 250 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.

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

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)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: ca.79 % - Readily biodegradable.
(ISO 14593)

12.3 Bioaccumulative potential

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

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

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 for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information**TDG**

UN number: 1175 Class: 3 Packing group: II
Proper shipping name: ETHYLBENZENE
Labels: 3
ERG Code: 130
Marine pollutant: no

IMDG

UN number: 1175 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ETHYLBENZENE

IATA

UN number: 1175 Class: 3 Packing group: II
Proper shipping name: Ethylbenzene

SECTION 15: Regulatory information

This product has been classified in accordance with the hazard criteria of the Hazardous Products Regulations (HPR) and the SDS contains all the information required by the HPR.

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

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