

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 27.06.2017

Version 12.1

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No. 801372

Product name Ethylbenzene for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 100-41-4

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

Identified uses Chemical for synthesis
For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0

Responsible Department LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number Please contact the regional company representation in your country.

SECTION 2. Hazards identification**2.1 Classification of the substance or mixture**

Classification (REGULATION (EC) No 1272/2008)

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Flammable liquid, Category 2, H225
Acute toxicity, Category 4, Inhalation, H332
Specific target organ toxicity - repeated exposure, Category 2, hearing organs, H373
Aspiration hazard, Category 1, H304
For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.
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.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P240 Ground/bond container and receiving equipment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P314 Get medical advice/ attention if you feel unwell.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H304 May be fatal if swallowed and enters airways.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

Index-No. 601-023-00-4

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	C ₆ H ₅ C ₂ H ₅	C ₈ H ₁₀ (Hill)
Index-No.	601-023-00-4	
EC-No.	202-849-4	
Molar mass	106,16 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
ethylbenzene (<= 100 %)		
100-41-4	*)	

Flammable liquid, Category 2, H225

Acute toxicity, Category 4, H332

Specific target organ toxicity - repeated exposure, Category 2,

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H373

Aspiration hazard, Category 1, H304

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

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Call a physician immediately. Pulmonary failure possible after aspiration of vomit.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Dermatitis, Drowsiness, Dizziness, narcosis, Nausea, Vomiting, Headache, Convulsions, Tiredness, CNS disorders
Drying-out effect resulting in rough and chapped skin.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

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Foam, Carbon dioxide (CO₂), Dry powder

Water, Foam, Carbon dioxide (CO₂), 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.

Vapours are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Special protective equipment 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.

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 vapours, 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.

Advice for emergency responders:

Protective equipment 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

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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

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

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.

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.

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

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8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Viton (R)
Glove thickness:	0,70 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 10 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 890 Vitoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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).

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Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur 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.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	characteristic
Odour Threshold	No information available.
pH	No information available.
Melting point	-95 °C
Boiling point/boiling range	136 °C at 1.013 hPa
Flash point	15 °C Method: c.c.

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Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,0 %(V)
Upper explosion limit	7,8 %(V)
Vapour pressure	9,5 hPa at 20 °C
Relative vapour density	3,66
Density	0,87 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,2 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,15 (25 °C) (experimental) (IUCLID) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	0,68 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

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9.2 Other data

Ignition temperature	430 °C
	Method: DIN 51794
Viscosity, kinematic	0,63 mm ² /s
	at 40 °C
	Method: ASTM D 445

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours 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

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 3.500 mg/kg

(IUCLID)

Acute inhalation toxicity

LC50 Rat: 17,2 mg/l; 4 h ; vapour

(IUCLID)

Symptoms: Irritation symptoms in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: 15.354 mg/kg

(IUCLID)

Skin irritation

Drying-out effect resulting in rough and chapped skin. Dermatitis

Eye irritation

This information is not available.

Sensitisation

Patch test: human

Result: negative

(IUCLID)

Germ cell mutagenicity

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Genotoxicity in vivo

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

Mouse

male and female

Inhalation

Result: negative

Method: OECD Test Guideline 474

Genotoxicity in vitro

Mutagenicity (mammal cell test):

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Mutagenicity (mammal cell test):

Result: negative

Method: OECD Test Guideline 479

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Target Organs: hearing organs

Repeated dose toxicity

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Rat
male and female
Oral
90 d
daily
NOAEL: 75 mg/kg
LOAEL: 250 mg/kg
OECD Test Guideline 408

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Further information

Systemic effects:

CNS disorders, Tiredness, Drowsiness, Dizziness, Convulsions, Headache, narcosis

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 *Oncorhynchus mykiss* (rainbow trout): 4,2 mg/l; 96 h

Analytical monitoring: yes

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

Analytical monitoring: yes

US-EPA

Toxicity to algae

EC50 *Pseudokirchneriella subcapitata* (green algae): 4,6 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

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Toxicity to bacteria

EC50 Photobacterium phosphoreum: 9,68 mg/l; 30 min

(IUCLID)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

semi-static test NOEC Ceriodaphnia dubia (water flea): 1 mg/l; 7 d

US-EPA

12.2 Persistence and degradability

Biodegradability

81 - 100 %; 14 d; aerobic

OECD Test Guideline 302C

Readily eliminated from water

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 3,15 (25 °C)

(experimental)

(IUCLID) Bioaccumulation is not expected.

12.4 Mobility in soil

Distribution among environmental compartments

Adsorption/Soil

log Koc: 2,31

(experimental)

Moderately mobile in soils (Lit.)

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

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

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

Land transport (ADR/RID)

14.1 UN number	UN 1175
14.2 Proper shipping name	ETHYLBENZENE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1175
14.2 Proper shipping name	ETHYLBENZENE
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

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Product name Ethylbenzene for synthesis

14.1 UN number UN 1175
14.2 Proper shipping name ETHYLBENZENE
14.3 Class 3
14.4 Packing group II
14.5 Environmentally hazardous --
14.6 Special precautions for user yes
EmS F-E S-D

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard SEVESO III
Legislation FLAMMABLE LIQUIDS
P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 3

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

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

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H332	Harmful if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

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Hazard statements

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Precautionary statements

Prevention

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240 Ground/bond container and receiving equipment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P314 Get medical advice/ attention if you feel unwell.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.