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Ethylbenzene ≥99 %, for synthesis

article number: **0272** Version: **GHS 4.0 en** Replaces version of: 2022-12-19 Version: (GHS 3)

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

1.1 Product identifier

Identification of the substance

Article number CAS number **Ethylbenzene** ≥99 %, for synthesis 0272

100-41-4

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

Relevant identified uses:

Uses advised against:

Laboratory chemical Laboratory and analytical use

Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 **e-mail:** sicherheit@carlroth.de **Website:** www.carlroth.de

Competent person responsible for the safety data Department Health, Safety and Environment sheet:

e-mail (competent person):

sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
NSW Poisons Information Centre Childrens Hospital	Hawkesbury Road	2145 West- mead, NSW	131126	

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
2.6	Flammable liquid	3	Flam. Liq. 3	H226
3.1I	Acute toxicity (inhal.)	4	Acute Tox. 4	H332
3.9	Specific target organ toxicity - repeated exposure	2	STOT RE 2	H373
3.10	Aspiration hazard	1	Asp. Tox. 1	H304

date of compilation: 2017-07-03 Revision: 2024-03-02

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For full text of abbreviations: see SECTION 16

The most important adverse physicochemical, human health and environmental effects

Delayed or immediate effects can be expected after short or long-term exposure. The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling

Signal word Danger

Pictograms

GHS08



Hazard statements

Flammable liquid and vapour
May be fatal if swallowed and enters airways
Harmful if inhaled
May cause damage to organs through prolonged or repeated exposure

Precautionary statements

Precautionary statements - prevention

P210	Keep away from heat/sparks/open flames/hot surfaces No smoking
P260	Do not breathe dust/fume/gas/mist/vapours/spray

Precautionary statements - response

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
P331	Do NOT induce vomiting
P370+P378	In case of fire: Use sand, carbon dioxide or powder extinguisher for extinction

Precautionary statements - storage

P403+P235 Store in a well-ventilated place. Keep cool

2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

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3.1

SECTION 3: Composition/information on ingredients

Substances	
Name of substance	Ethylbenzene
Molecular formula	C ₈ H ₁₀
Molar mass	106.1 ^g / _{mol}
CAS No	100-41-4

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

Following ingestion

Call a physician immediately. Observe aspiration hazard if vomiting occurs.

4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Vertigo, Headache, Dizziness, Spasms, Nausea, Vomiting, Aspiration hazard

4.3 Indication of any immediate medical attention and special treatment needed none

SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet



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5.2 Special hazards arising from the substance or mixture

Combustible. In case of insufficient ventilation and/or in use, may form flammable/explosive vapourair mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains.

Advice on how to clean up a spill

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

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Take precautionary measures against static discharge.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ground/bond container and receiving equipment.

Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation.

Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Cou ntr y	Name of agent	CAS No	Identi- fier	TW A [pp m]	TWA [mg/ m³]	STE L [pp m]	STEL [mg/ m³]	Ceil ing- C [pp m]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
AU	ethylbenzene	100-41-4	WES	100	434	125	543				WES

Notation

TWA

Ceiling-C Ceiling value is a limit value above which exposure should not occur STEL Short-term exposure limit: a limit value above which exposure shoul

Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15minute period (unless otherwise specified)

Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average (unless otherwise specified)

Human health values

Relevant DNELs and other threshold levels					
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time	
DNEL	77 mg/m³	human, inhalatory	worker (industry)	chronic - systemic effects	
DNEL	293 mg/m³	human, inhalatory	worker (industry)	acute - local effects	

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Relevant DNELs and other threshold levels					
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time	
DNEL	180 mg/kg bw/ day	human, dermal	worker (industry)	chronic - systemic effects	

Environmental values

Relevant PNECs and other threshold levels						
End- point	Threshold level	Organism	Environmental com- partment	Exposure time		
PNEC	0.1 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)		
PNEC	0.01 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)		
PNEC	9.6 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)		
PNEC	13.7 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)		
PNEC	1.37 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)		
PNEC	2.68 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)		

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a consider-able reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

• type of material

FKM: fluoro-elastomer

material thickness

0,4 mm

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• breakthrough times of the glove material

- >480 minutes (permeation: level 6)
- Splash protection Protective gloves
- type of material: NBR (Nitrile rubber)
- material thickness: 0,4 mm
- breakthrough times of the glove material:

other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

>10 minutes (permeation: level 1)

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C , colour code: Brown).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	characteristic
Melting point/freezing point	-94.9 °C at 1,013 hPa (ECHA)
Boiling point or initial boiling point and boiling range	136.1 °C at 1,013 hPa (ECHA)
Flammability	flammable liquid in accordance with GHS criteria
Lower and upper explosion limit	43 g/m³ (LEL) - 340 g/m³ (UEL) / 1 vol% (LEL) - 7.8 vol% (UEL)
Flash point	23 °C at 1,013 hPa (ECHA)
Auto-ignition temperature	430 °C at 1,013 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	0.773 ^{mm²} / _s at 20 °C
Dynamic viscosity	0.6725 cP at 20 °C
Solubility(ies)	
Water solubility	0.2 ^g / _l at 25 °C (ECHA)
Partition coefficient	
Partition coefficient n-octanol/water (log value):	3.6 (pH value: 7.84, 20 °C) (ECHA)



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	Vapour pressure	9.52 hPa at 20 °C
	Density and/or relative density	
	Density	0.87 ^g / _{cm³} at 20 °C
	Relative vapour density	3.67 (air = 1)
	Particle characteristics Other safety parameters	not relevant (liquid)
	Oxidising properties	none
9.2	Other information	
	Information with regard to physical hazard classes:	There is no additional information.
	Other safety characteristics:	
	Surface tension	71.2 ^{mN} / _m (23 °C) (ECHA)

SECTION 10: Stability and reactivity

10.1 Reactivity

It's a reactive substance. Risk of ignition. Vapours may form explosive mixtures with air.

If heated

Risk of ignition.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

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

10.5 Incompatible materials

Rubber articles, different plastics

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if inhaled.

GHS of the United Nations, annex 4. May be harmful if swallowed.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	3,500 ^{mg} / _{kg}	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

May be fatal if swallowed and enters airways.

Symptoms related to the physical, chemical and toxicological characteristics

If swallowed

vomiting, aspiration hazard

• If in eyes

Data are not available.

• If inhaled

irritant effects

• If on skin

Data are not available.

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Other information

Other adverse effects: Headache, Spasms, Nausea, Vertigo, Dizziness

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (ac	Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time	
LC50	5.1 ^{mg} / _l	fish	ECHA	96 h	
EC50	2.4 ^{mg} / _l	aquatic invertebrates	ECHA	48 h	

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
LC50	3.6 ^{mg} / _l	aquatic invertebrates	ECHA	7 d

12.2 Persistence and degradability

Theoretical Oxygen Demand: 3.167 ^{mg}/_{mg} Theoretical Carbon Dioxide: 3.318 ^{mg}/_{mg}

Biodegradation

The substance is readily biodegradable.

Process of degradability				
Process	Degradation rate	Time		
biotic/abiotic	79 %	28 d		

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n	n-octanol/water (log KOW)	3.6 (pH value: 7.84, 20 °C) (ECHA)
E	3CF	1 (ECHA)

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.



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12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

Relevant provisions relating to waste(Basel Convention)

Properties of waste which render it hazardous

H3 Flammable liquids

H11 Toxic (Delayed or chronic)

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

SECTION 14: Transport information

14.1	UN	num	ber
------	----	-----	-----

	UN RTDG	UN 1175
	IMDG-Code	UN 1175
	ICAO-TI	UN 1175
14.2	UN proper shipping name	
	UN RTDG	ETHYLBENZENE
	IMDG-Code	ETHYLBENZENE
	ICAO-TI	Ethylbenzene
14.3	Transport hazard class(es)	
	UN RTDG	3
	IMDG-Code	3
	ICAO-TI	3
14.4	Packing group	
	UN RTDG	II
	IMDG-Code	II

Safety data sheet Safety data sheet acc. to Safe Work Australia - Code of Practice



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	ICAO-TI	II
14.5	Environmental hazards	non-environmentally hazardous acc. to the dan- gerous goods regulations
14.6	Special precautions for user There is no additional information.	
14.7	Transport in bulk according to IMO instrument The cargo is not intended to be carried in bulk.	S
14.8	Information for each of the UN Model Regulation	ons
	Transport informationNational regulationsAdd	itional information(UN RTDG)
	UN number	1175
	Class	3
	Packing group	II
	Danger label(s)	3
	Special provisions (SP)	- UN RTDG
	Excepted quantities (EQ)	E2 UN RTDG
	Limited quantities (LQ)	1 L UN RTDG
	Emergency Action Code	3YE
	International Maritime Dangerous Goods Code	(IMDG) - Additional information
	Proper shipping name	ETHYLBENZENE
	Particulars in the shipper's declaration	UN1175, ETHYLBENZENE, 3, II, 23°C c.c.
	Marine pollutant	-
	Danger label(s)	3
	Special provisions (SP)	-
	Excepted quantities (EQ)	E2
	Limited quantities (LQ)	1 L
	EmS	F-E, S-D
	Stowage category	В

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International Civil Aviation Organization (ICA	AO-IATA/DGR) - Additional information
Proper shipping name	Ethylbenzene
Particulars in the shipper's declaration	UN1175, Ethylbenzene, 3, II
Danger label(s)	3
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture 15.1 There is no additional information.

National regulations(Australia)

Australian Inventory of Chemical Substances(AICS)

Substance is listed.

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend AIIČ

CICR

DSL ECSI

IECSC

Australian Inventory of Industrial Chemicals Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS) CSCL-ENCS

Environ Existing and the content and a balances (CSCE Ences), EC Substances List (DSL) EC Substance Inventory (EINECS, ELINCS, NLP) Inventory of Existing Chemical Substances Produced or Imported in China

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Legend	
INSQ National Inventory of Chemical Substances	
KECI Korea Existing Chemicals Inventory	
NCI National Chemical Inventory	
NZIoC New Zealand Inventory of Chemicals	
PICCS Philippine Inventory of Chemicals and Chemical Substance	ces (PICCS)
REACH Reg. REACH registered substances	
TCSI Taiwan Chemical Substance Inventory	
TSCA Toxic Substance Control Act	

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
15.1		National inventories: change in the listing (table)	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Na- tions
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code

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Abbr.	Descriptions of used abbreviations
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
ppm	Parts per million
STEL	Short-term exposure limit
TWA	Time-weighted average
UEL	Upper explosion limit (UEL)
UN RTDG	UN Recommendations on the Transport of Dangerous Good
vPvB	Very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne contaminants

Key literature references and sources for data

Safe Work Australia's Code of Practice for Labelling of Workplace Hazardous Chemicals (under WHS Regulations).

UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H226	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.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.