

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester \geq 99%, for synthesis

article number: **4368**
Version: **2.0 en**
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Version: (1)

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Revision: 2022-05-06

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

1.1 Product identifier

Identification of the substance	Acetic acid benzyl ester \geq 99%, for synthesis
Article number	4368
Registration number (REACH)	01-2119638272-42-xxxx
EC number	205-399-7
CAS number	140-11-4

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household).

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 sheet: Department Health, Safety and Environment

e-mail (competent person): sicherheit@carlroth.de

1.4 Emergency telephone number

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Centre Beaumont Hospital	Beaumont Road	Dublin 9	01 809 2166	https://www.poisons.ie/

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
4.1C	Hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

For full text of abbreviations: see SECTION 16

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

The most important adverse physicochemical, human health and environmental effects

Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word Not required

Not required

Pictograms

Hazard statements

H412 Harmful to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P273 Avoid release to the environment

Labelling of packages where the contents do not exceed 125 ml

Signal word: Not required.

H412 Harmful to aquatic life with long lasting effects.

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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Acetic acid benzyl ester
Molecular formula	$C_9H_{10}O_2$
Molar mass	150,2 g/mol
REACH Reg. No	01-2119638272-42-xxxx
CAS No	140-11-4
EC No	205-399-7

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.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

Following skin contact

Rinse skin with water/shower.

Following eye contact

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

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Irritant effects, Headache, Dizziness, Vomiting

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

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and 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. Do not allow firefighting water to enter drains or water courses. 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

Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

6.2 Environmental precautions

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

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

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.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

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:

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)

Country	Name of agent	CAS No	Identifier	TW A [ppm]	TWA [mg/m ³]	STE L [ppm]	STEL [mg/m ³]	Ceiling-C [ppm]	Ceiling-C [mg/m ³]	Notation	Source
IE	benzyl acetate	140-11-4	OELV		10						S.I. No. 619 of 2001

Notation

Ceiling-C
STEL

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

TWA

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)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	9 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	2,5 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 compartment	Exposure time
PNEC	0,018 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,002 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	8,55 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,526 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,053 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,094 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 considerable 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

Butyl caoutchouc (butyl rubber)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

- **material thickness**

0,7mm

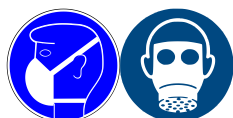
- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

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

Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of $> 65\text{ }^{\circ}\text{C}$, 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	clear
Odour	characteristic
Melting point/freezing point	$-51,5\text{ }^{\circ}\text{C}$ (ECHA)
Boiling point or initial boiling point and boiling range	$213,5\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	0,9 vol% (LEL) - 8,4 vol% (UEL)
Flash point	$102\text{ }^{\circ}\text{C}$ at 1.013 hPa (c.c.) (ECHA)
Auto-ignition temperature	$460\text{ }^{\circ}\text{C}$ at 1.013 Pa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	$4,269\text{ mm}^2/\text{s}$ at $25\text{ }^{\circ}\text{C}$
Dynamic viscosity	$4,5\text{ mPa s}$ at $25\text{ }^{\circ}\text{C}$
<u>Solubility(ies)</u>	
Water solubility	$<1\text{ g/l}$ at $20\text{ }^{\circ}\text{C}$ (poorly soluble)
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	1,96 (pH value: 7, $25\text{ }^{\circ}\text{C}$) (ECHA)
Soil organic carbon/water (log KOC)	2,4 (ECHA)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

Vapour pressure 0,24 hPa at 25 °C

Density and/or relative density

Density 1,054 g/cm³ at 25 °C (ECHA)

Relative vapour density 5,19 (air = 1)

Particle characteristics not relevant (liquid)

Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

Temperature class (EU, acc. to ATEX) T1
Maximum permissible surface temperature on the equipment: 450°C

SECTION 10: Stability and reactivity

10.1 Reactivity

This material is not reactive under normal ambient conditions.

If heated

Vapours may form explosive mixtures with air.

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.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

SECTION 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	$>2.000 \text{ mg/kg}$	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

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

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

vomiting

• If in eyes

slightly irritant but not relevant for classification

• If inhaled

slightly irritant but not relevant for classification

• If on skin

slightly irritant but not relevant for classification

• Other information

none

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

11.2 Endocrine disrupting properties

Not listed.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	4 mg/l	fish	ECHA	96 h
EC50	25 mg/l	aquatic invertebrates	ECHA	24 h
ErC50	110 mg/l	algae	ECHA	72 h

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	855 mg/l	microorganisms	ECHA	3 h

Biodegradation

The substance is readily biodegradable.

12.2 Process of degradability

Theoretical Oxygen Demand: 2,237 mg/mg
Theoretical Carbon Dioxide: 2,637 mg/mg

Process of degradability		
Process	Degradation rate	Time
carbon dioxide generation	100,9 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,96 (pH value: 7, 25 °C) (ECHA)
BCF	8 (ECHA)

12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2,4 (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

12.6 Endocrine disrupting properties

Not listed.

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. Avoid release to the environment. Refer to special instructions/safety data sheets.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process. Waste catalogue ordinance (Germany).

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.

SECTION 14: Transport information

- | | |
|--|---|
| 14.1 UN number or ID number | not subject to transport regulations |
| 14.2 UN proper shipping name | not assigned |
| 14.3 Transport hazard class(es) | none |
| 14.4 Packing group | not assigned |
| 14.5 Environmental hazards | non-environmentally hazardous acc. to the dangerous goods regulations |
| 14.6 Special precautions for user | There is no additional information. |
| 14.7 Maritime transport in bulk according to IMO instruments | The cargo is not intended to be carried in bulk. |
| 14.8 <u>Information for each of the UN Model Regulations</u> | |
| Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information | Not subject to ADR, RID and ADN. |
| International Maritime Dangerous Goods Code (IMDG) - Additional information | Not subject to IMDG. |
| International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information | Not subject to ICAO-IATA. |

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester \geq 99%, for synthesis

article number: 4368

SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

Dangerous substances with restrictions (REACH, Annex XVII)				
Name of substance	Name acc. to inventory	CAS No	Restriction	No
Acetic acid benzyl ester	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		R3	3

Legend

- R3
1. Shall not be used in:
 - ornamental articles intended to produce light or colour effects by means of different phases, for example in ornamental lamps and ashtrays,
 - tricks and jokes,
 - games for one or more participants, or any article intended to be used as such, even with ornamental aspects,
 2. Articles not complying with paragraph 1 shall not be placed on the market.
 3. Shall not be placed on the market if they contain a colouring agent, unless required for fiscal reasons, or perfume, or both, if they:
 - can be used as fuel in decorative oil lamps for supply to the general public, and
 - present an aspiration hazard and are labelled with H304.
 4. Decorative oil lamps for supply to the general public shall not be placed on the market unless they conform to the European Standard on Decorative oil lamps (EN 14059) adopted by the European Committee for Standardisation (CEN).
 5. Without prejudice to the implementation of other Union provisions relating to the classification, labelling and packaging of substances and mixtures, suppliers shall ensure, before the placing on the market, that the following requirements are met:
 - (a) lamp oils, labelled with H304, intended for supply to the general public are visibly, legibly and indelibly marked as follows: "Keep lamps filled with this liquid out of the reach of children"; and, by 1 December 2010, "Just a sip of lamp oil – or even sucking the wick of lamps – may lead to life-threatening lung damage";
 - (b) grill lighter fluids, labelled with H304, intended for supply to the general public are legibly and indelibly marked by 1 December 2010 as follows: "Just a sip of grill lighter fluid may lead to life threatening lung damage";
 - (c) lamps oils and grill lighters, labelled with H304, intended for supply to the general public are packaged in black opaque containers not exceeding 1 litre by 1 December 2010.;

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list

Not listed.

Seveso Directive

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

Deco-Paint Directive

VOC content	100 % 1.054 g/l
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Industrial Emissions Directive (IED)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester $\geq 99\%$, for synthesis

article number: 4368

VOC content	100 %
VOC content	1.054 g/l

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

not listed

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not 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

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester ≥ 99%, for synthesis

article number: 4368

Legend

AIIC	Australian Inventory of Industrial Chemicals
CICR	Chemical Inventory and Control Regulation
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (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)

Alignment to regulation: Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU

Restructuring: section 9, section 14

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.1		Classification according to Regulation (EC) No 1272/2008 (CLP): change in the listing (table)	yes
2.1		The most important adverse physicochemical, human health and environmental effects: Spillage and fire water can cause pollution of watercourses.	yes
2.2		Pictograms: Not required	yes
2.3	Other hazards: There is no additional information.	Other hazards	yes
2.3		Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester \geq 99%, for synthesis

article number: 4368

Abbr.	Descriptions of used abbreviations
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
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ErC50	\equiv EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
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
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
S.I. No. 619 of 2001	Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
UEL	Upper explosion limit (UEL)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.
Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH)



Acetic acid benzyl ester \geq 99%, for synthesis

article number: **4368**

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

Code	Text
H412	Harmful to aquatic life with long lasting effects.

Disclaimer

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