

## Acetic acid isobutyl ester ≥99 %, for synthesis

article number: **4370**  
Version: **GHS 1.0 en**

date of compilation: 2016-04-25

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

#### 1.1 Product identifier

Identification of the substance	<b>Acetic acid isobutyl ester</b>
Article number	4370
Registration number (REACH)	01-2119488971-22-xxxx
Index No	607-026-00-7
EC number	203-745-1
CAS number	110-19-0

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

**Identified uses:** laboratory chemical

#### 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](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

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

**e-mail (competent person)** : [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

#### 1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

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

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquid	(Flam. Liq. 2)	H225
3.3	serious eye damage/eye irritation	(Eye Irrit. 2)	H319
3.8D	specific target organ toxicity - single exposure (narcotic effects, drowsiness)	(STOT SE 3)	H336

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according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



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### Supplemental hazard information

Code	Supplemental hazard information
EUH066	repeated exposure may cause skin dryness or cracking

#### Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

### The most important adverse physicochemical, human health and environmental effects

Narcotic effects.

## 2.2 Label elements

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

**Signal word**                      **Danger**

#### Pictograms



#### Hazard statements

H225                      Highly flammable liquid and vapour.  
H319                      Causes serious eye irritation.  
H336                      May cause drowsiness or dizziness.

#### Precautionary statements

##### **Precautionary statements - prevention**

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

##### **Precautionary statements - response**

P305+P351+P338      IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P312                      Call a POISON CENTER/doctor if you feel unwell.  
P370+P378              In case of fire: Use sand, carbon dioxide or powder extinguisher to extinguish.

##### **Precautionary statements - storage**

P403+P233              Store in a well-ventilated place. Keep container tightly closed.  
P403+P235              Store in a well-ventilated place. Keep cool.

##### **Precautionary statements - disposal**

P501                      Dispose of contents/container to industrial combustion plant.

### Supplemental hazard information

EUH066                      Repeated exposure may cause skin dryness or cracking.

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### Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



EUH066

Repeated exposure may cause skin dryness or cracking.

### 2.3 Other hazards

There is no additional information.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Acetic acid isobutyl ester
Index No	607-026-00-7
Registration number (REACH)	01-2119488971-22-xxxx
EC number	203-745-1
CAS number	110-19-0
Molecular formula	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>
Molar mass	116.2 g/mol

## 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. Frequently or prolonged contact with skin may cause dermal irritation. In case of skin reactions, consult a physician.

#### Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

#### Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

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### 4.2 Most important symptoms and effects, both acute and delayed

Irritation, Irritant effects, Dyspnoea, Dizziness, Drowsiness, Narcosis

### 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 fire-fighting measures to the fire surroundings  
water spray, foam, alcohol resistant foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

#### 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. Vapours can form explosive mixtures with air.

#### Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

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

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. 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. Explosive properties.

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

#### Advices on how to contain a spill

Covering of drains.

#### Advices on how to clean up a spill

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

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

#### 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.

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### 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.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

#### 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

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)

Country	Name of agent	CAS No	Notation	Identifier	TWA [ppm]	TWA [mg/m <sup>3</sup> ]	STEL [ppm]	STEL [mg/m <sup>3</sup> ]	Source
AU	isobutyl acetate	110-19-0		WES	150	713			WES

##### Notation

STEL 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

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### Relevant DNELs/DMELs/PNECs and other threshold levels

#### • human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	300 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - local effects
DNEL	600 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	acute - local effects
DNEL	10 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects
DNEL	10 mg/kg bw/day	human, dermal	worker (industry)	acute - systemic effects

#### • environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0.17 mg/l	freshwater	short-term (single instance)
PNEC	0.017 mg/l	marine water	short-term (single instance)
PNEC	0.34 mg/l	water	continuous
PNEC	200 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	0.877 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0.088 mg/kg	marine sediment	short-term (single instance)
PNEC	0.075 mg/kg	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.

##### • type of material

Butyl caoutchouc (butyl rubber)

##### • material thickness

0,7mm.

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- **breakthrough times of the glove material**

>60 minutes (permeation: level 3), >480 minutes (permeation: level 6)

- **other protection measures**

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

Flame-retardant protective clothing.

### 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

#### Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	fruity
Odour threshold	4.05 ppm

#### Other physical and chemical parameters

pH (value)	5 (water: 4 g/l, 20 °C)
Melting point/freezing point	<-90 °C
Initial boiling point and boiling range	117 °C at 1,013 hPa
Flash point	22 °C at 1,013 hPa (closed cup)
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	1.3 vol% (60 g/m <sup>3</sup> )
• upper explosion limit (UEL)	10.5 vol% (510 g/m <sup>3</sup> )
Explosion limits of dust clouds	not relevant
Vapour pressure	21 hPa at 20 °C 89 hPa at 50 °C
Density	0.871 g/cm <sup>3</sup> at 20 °C
Vapour density	4.01 at 20 °C (air = 1)
Bulk density	Not applicable
Relative density	Information on this property is not available.

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### Solubility(ies)

Water solubility 5.6 g/l at 20 °C

### Partition coefficient

n-octanol/water (log KOW) 2.3 (pH value: 7, 25 °C) (ECHA)

Auto-ignition temperature 430 °C - ECHA

Decomposition temperature no data available

### Viscosity

• dynamic viscosity 0.699 mPa s at 20 °C

Explosive properties none

Oxidising properties none

## 9.2 Other information

Surface tension 62.5 mN/m (20 °C)

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

risk of ignition. Vapours can 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

Exothermic reaction with: Oxidisers,  
Danger of explosion: Alkali hydroxide<sup>-</sup> (caustic alkali)

### 10.4 Conditions to avoid

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

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	13,413 mg/kg	rat	ECHA
dermal	LD50	>17,400 mg/kg	rabbit	ECHA



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### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

### Serious eye damage/eye irritation

Causes serious eye irritation.

### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

#### • Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

#### • 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, nausea

#### • If in eyes

slightly irritant but not relevant for classification

#### • If inhaled

breathing difficulties, fatigue, narcosis

#### • If on skin

Frequently or prolonged contact with skin may cause dermal irritation

### Other information

None

## SECTION 12: Ecological information

### 12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

#### Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	16.6 mg/l	fish	ECHA	96 hours
EC50	24.6 mg/l	aquatic invertebrates	ECHA	48 hours
ErC50	392 mg/l	algae	ECHA	48 hours

#### Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	34.2 mg/l	aquatic invertebrates	ECHA	21 d
LC50	43.5 mg/l	aquatic invertebrates	ECHA	21 d
ErC50	335 mg/l	algae	ECHA	24 h
NOEC	23.2 mg/l	aquatic invertebrates	ECHA	21 d

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Endpoint	Value	Species	Source	Exposure time
LOEC	47.6 mg/l	aquatic invertebrates	ECHA	21 d

### 12.2 Process of degradability

The substance is readily biodegradable.  
Theoretical Oxygen Demand: 2.204 mg/mg  
Theoretical Carbon Dioxide: 2.273 mg/mg

Process	Degradation rate	Time
oxygen depletion	81 %	20 d

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

2.3 (pH value: 7, 25 °C)

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Other adverse effects

Slightly hazardous to water.

## 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

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

### 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.

### 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.

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### SECTION 14: Transport information

<b>14.1</b>	UN number	<b>1213</b>
<b>14.2</b>	UN proper shipping name	<b>ISOBUTYL ACETATE</b>
	Hazardous ingredients	Acetic acid isobutyl ester
<b>14.3</b>	Transport hazard class(es)	
	Class	3 (flammable liquids)
<b>14.4</b>	Packing group	II (substance presenting medium danger)
<b>14.5</b>	Environmental hazards	none (non-environmentally hazardous acc. to the dangerous goods regulations)
<b>14.6</b>	<b>Special precautions for user</b>	
	Provisions for dangerous goods (ADR) should be complied within the premises.	
<b>14.7</b>	<b>Transport in bulk according to Annex II of MARPOL and the IBC Code</b>	
	The cargo is not intended to be carried in bulk.	
<b>14.8</b>	<b>Information for each of the UN Model Regulations</b>	
	<b>• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)</b>	
	UN number	1213
	Proper shipping name	ISOBUTYL ACETATE
	Particulars in the transport document	UN1213, ISOBUTYL ACETATE, 3, II, (D/E)
	Class	3
	Classification code	F1
	Packing group	II
	Danger label(s)	3
		
	Excepted quantities (EQ)	E2
	Limited quantities (LQ)	1 L
	Transport category (TC)	2
	Tunnel restriction code (TRC)	D/E
	Hazard identification No	33
	<b>Emergency Action Code</b>	3YE
	<b>• International Maritime Dangerous Goods Code (IMDG)</b>	
	UN number	1213
	Proper shipping name	ISOBUTYL ACETATE
	Particulars in the shipper's declaration	UN1213, ISOBUTYL ACETATE, 3, II, 22°C c.c.
	Class	3
	Packing group	II



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### Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II

not listed

### Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

### Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

## 15.2 Chemical Safety Assessment

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

## SECTION 16: Other information

### 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 européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
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 Nations
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
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

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Abbr.	Descriptions of used abbreviations
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
STEL	short-term exposure limit
TWA	time-weighted average
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative
WES	Safe Work Australia: Workplace exposure standards for airborne conatminants

### Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

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

Code	Text
H225	highly flammable liquid and vapour
H319	causes serious eye irritation
H336	may cause drowsiness or dizziness

### Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.