

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis

article number: **1PKX**  
Version: **2.0 en**  
Replaces version of: 2022-06-02  
Version: (1)

date of compilation: 2022-06-02  
Revision: 2024-03-02

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

### 1.1 Product identifier

Identification of the substance	<b>3-Methoxy-3-methylbutyl acetate</b> ≥98 % for synthesis
Article number	1PKX
EC number	700-408-5
CAS number	103429-90-9
Alternative name(s)	3-Methoxy-3-methylbutyl acetate

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

Relevant identified uses:	Laboratory and analytical use Laboratory chemical
Uses advised against:	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](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

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification acc. to GHS

This substance does not meet the criteria for classification.

### 2.2 Label elements

#### Labelling

not required

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98\%$ for synthesis

article number: **1PKX**

### 2.3 Other hazards

This material is combustible, but will not ignite readily.

#### 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  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	3-Methoxy-3-methylbutyl acetate
Molecular formula	$C_8H_{16}O_3$
Molar mass	160,2 $g/mol$
CAS No	103429-90-9
EC No	700-408-5

## 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

Rinse mouth. Call a doctor if you feel unwell.

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

Symptoms and effects are not known to date.

### 4.3 Indication of any immediate medical attention and special treatment needed

none

# Safety data sheet

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



**3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis**

article number: **1PKX**

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water spray, alcohol resistant foam, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible.

#### Hazardous combustion products

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

### 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

No special measures are necessary.

### 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.

#### 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.

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98\%$ for synthesis

article number: 1PKX

### 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.

#### Advice on general occupational hygiene

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)

This information is not available.

##### Human health values

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	2,47 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,7 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	73,8 $\mu\text{g}/\text{l}$	aquatic organisms	freshwater	short-term (single instance)
PNEC	7,38 $\mu\text{g}/\text{l}$	aquatic organisms	marine water	short-term (single instance)

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98$ % for synthesis

article number: **1PKX**

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	10 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,38 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	38,3 $\mu$ g/kg	aquatic organisms	marine sediment	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.

##### • type of material

Butyl caoutchouc (butyl rubber)

##### • material thickness

>0,11 mm

##### • 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 °C , colour code: Brown).

##### Environmental exposure controls

Keep away from drains, surface and ground water.

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis

article number: **1PKX**

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	transparent
Odour	acc. to product description
Melting point/freezing point	-100 – 25 °C at 1.013 hPa (ECHA)
Boiling point or initial boiling point and boiling range	187,3 °C at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	76 °C at 1.008 mbar (ECHA)
Auto-ignition temperature	>400 °C at 1.008 mbar (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined

#### Solubility(ies)

Water solubility 58,3 g/l at 20 °C (ECHA)

#### Partition coefficient

Partition coefficient n-octanol/water (log value): 1,6 (pH value: ~7, 25 °C) (ECHA)

Soil organic carbon/water (log KOC) 1,2 (ECHA)

Vapour pressure 258 Pa at 25 °C

#### Density and/or relative density

Density 0,957 g/cm<sup>3</sup> at 20 °C (ECHA)

Relative vapour density Information on this property is not available.

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:

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis

article number: **1PKX**

Surface tension

65,5 mN/m (20 °C) (ECHA)

### 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, 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

##### Classification acc. to GHS

This substance does not meet the criteria for classification.

##### Acute toxicity

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful if swallowed or in contact with skin.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	4.600 mg/kg	rat		ECHA
dermal	LD50	>2.000 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.

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98$ % for synthesis

article number: **1PKX**

### **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**

Data are not available.

#### **• If in eyes**

Data are not available.

#### **• If inhaled**

Data are not available.

#### **• If on skin**

Data are not available.

#### **• Other information**

Health effects are not known.

### **11.2 Endocrine disrupting properties**

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

### **11.3 Information on other hazards**

There is no additional information.

## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Shall not be classified as hazardous to the aquatic environment.

<b>Aquatic toxicity (acute)</b>				
<b>Endpoint</b>	<b>Value</b>	<b>Species</b>	<b>Source</b>	<b>Exposure time</b>
LC50	84,9 mg/l	fish	ECHA	48 h
EC50	>100 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	>100 mg/l	algae	ECHA	72 h



# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98\%$ for synthesis

article number: 1PKX

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	$>1.000 \text{ mg/l}$	microorganisms	ECHA	3 h

### 12.2 Persistence and degradability

Theoretical Oxygen Demand:  $2,097 \text{ mg/mg}$   
Theoretical Carbon Dioxide:  $2,198 \text{ mg/mg}$

#### Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	90 %	28 d
DOC removal	97 %	28 d

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,6 (pH value: $\sim 7$ , $25^\circ\text{C}$ ) (ECHA)
---------------------------	---

### 12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	1,2 (ECHA)
--	------------

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

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

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

#### Sewage disposal-relevant information

Do not empty into drains.

#### Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98$ % for synthesis

article number: **1PKX**

### 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. Non-contaminated packages may be recycled.

## 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 Information for each of the UN Model Regulations**
- 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.

## 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)**

#### 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

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis

article number: **1PKX**

VOC content	100 %
VOC content	957 g/l

### Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	957 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

### National regulations(GB)

#### List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

#### Restrictions according to GB REACH, Annex 17

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
CN	IECSC	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
JP	ISHA-ENCS	substance is listed

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate ≥98 % for synthesis

article number: **1PKX**

Country	Inventory	Status
KR	KECI	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

### Legend

CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
ISHA-ENCS	Inventory of Existing and New Chemical Substances (ISHA-ENCS)
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
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)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	VOC content: 100 % 957 g/l	VOC content: 100 %	yes
15.1		VOC content: 957 g/l	yes
15.1		National inventories: change in the listing (table)	yes

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
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

# Safety data sheet

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



## 3-Methoxy-3-methylbutyl acetate $\geq 98$ % for synthesis

article number: **1PKX**

Abbr.	Descriptions of used abbreviations
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)
ED	Endocrine disruptor
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
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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)
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

### Key literature references and sources for data

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).

### Disclaimer

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