

# Voluntary safety information following the Safety Data Sheet format according 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
Registration number (REACH)	01-2119847299-23-xxxx
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 Centre Beaumont Hospital	Beaumont Road	Dublin 9	+353 1 809 2166	<a href="https://www.poisons.ie/">https://www.poisons.ie/</a>

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

article number: 1PKX

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

### 2.2 Label elements

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

not required

### 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 $g/mol$
REACH Reg. No	01-2119847299-23-xxxx
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.

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

article number: 1PKX

**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

## 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.

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

article number: 1PKX

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.

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

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

article number: 1PKX

**Environmental values**

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	73,8 µg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	7,38 µg/l	aquatic organisms	marine water	short-term (single instance)
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 µg/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).

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

article number: 1PKX

**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	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
<u>Solubility(ies)</u>	
Water solubility	58,3 g/l at 20 °C (ECHA)
<u>Partition coefficient</u>	
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
<u>Density and/or relative density</u>	
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)
<u>Other safety parameters</u>	
Oxidising properties	none

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

article number: 1PKX

#### 9.2 Other information

Information with regard to physical hazard classes:

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

Other safety characteristics:

Surface tension

65,5 mN/m (20 °C) (ECHA)

Temperature class (EU, acc. to ATEX)

T2  
Maximum permissible surface temperature on the equipment: 300°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, 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 hazard classes as defined in Regulation (EC) No 1272/2008

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

#### Acute toxicity

Shall not be classified as acutely toxic.

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.

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

article number: **1PKX**

---

**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**

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.



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

article number: 1PKX

## SECTION 12: Ecological information

### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
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

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

### 12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,097 mg/mg  
Theoretical Carbon Dioxide: 2,198 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: ~7, 25 °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 ≥ 0,1%.

### 12.7 Other adverse effects

Data are not available.

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

article number: 1PKX

## 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.

### 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 <u>Information for each of the UN Model Regulations</u>                              |   |
| <b>International Maritime Dangerous Goods Code (IMDG) - Additional information</b>        | Not subject to IMDG.  |
| <b>International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information</b> | Not subject to ICAO-IATA.   |

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

article number: 1PKX

## 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

not listed

##### 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 %
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

# Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)



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

article number: **1PKX**

### 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
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

According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.

## 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

**Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)**



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

article number: **1PKX**

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
15.1		National inventories: change in the listing (table)	yes
15.2	Chemical Safety Assessment: No Chemical Safety Assessment has been carried out for this substance.	Chemical safety assessment: According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.	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)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
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
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	≡ 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
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals

# Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)



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

article number: **1PKX**

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)
SVHC	Substance of Very High Concern
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).

### Disclaimer

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