

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

# tert-Butyl acetoacetate

Version number: 1

Issued: 2024-02-05



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

### 1.1. Product identifier

**Trade name**

tert-Butyl acetoacetate

**CAS number**

1694-31-1

**EC number**

216-904-5

**Synonyms**

tert-butyl 3-oxobutanoate

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

**Relevant identified uses**

Research and development. Laboratory Chemicals. Manufacture of substances.

**Not suitable for use in**

Not suitable for human consumption or veterinary purposes.

### 1.3. Details of the supplier of the safety data sheet

**Supplier**

Molekula Group

**Address**

Molekula Ltd, Lingfield Way, Darlington,  
DL1 4XX Darlington  
United Kingdom

**Telephone**

+44 (0) 3302 000 333

**Email**

info@molekula.com

**Web site**

www.molekula.com

**Contact person**

Kevin Banks

**Email**

+44 (0) 7769276927

### 1.4. Emergency telephone number

**Poison center/Additional emergency number**

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

The product is not classified as hazardous according to Regulation (EC) No 1272/2008.

### 2.2. Label elements

#### Precautionary statements

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P314 Get medical advice/attention if you feel unwell.

P362 + P364 Take off contaminated clothing and wash it before reuse.

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

P405 Store locked up.

P501 Dispose of contents/container to local regulations.

### 2.3. Other hazards

No data available

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
tert-Butyl acetoacetate	1694-31-1 216-904-5 - -	100%	-	- - -	-

#### Molecular weight

158.19

#### Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

#### Inhalation

Move to fresh air if inhaled.

Get medical attention if any discomfort continues.

#### Skin contact

Rinse skin with water.

If skin irritation or rash occurs: Get medical advice/attention.

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## **Eye contact**

Remove contact lenses if present. Rinse eyes with water.  
If eye irritation persists: Get medical advice/attention.

## **Ingestion**

Rinse mouth.  
Get medical advice/attention if you feel unwell.

## **Information for doctors**

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

## **Inhalation**

May cause respiratory irritation.

## **Skin contact**

Prolonged contact may cause dryness of the skin.

## **Eye contact**

May be slightly irritating to the eyes.

## **Ingestion**

May cause discomfort if swallowed.

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

Treat symptomatically. No special treatment requirement.

## **SECTION 5: Firefighting measures**

### **5.1. Extinguishing media**

#### **Suitable extinguishing media**

Foam, carbon dioxide or dry powder.

#### **Unsuitable extinguishing media**

No specific fire fighting procedure given.

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

Specific hazards: None.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

Vapours are heavier than air and may travel along the floor and in the bottom of containers.

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## 5.3. Advice for firefighters

### Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. For personal protection, see section 8.

### 6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

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

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

### 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Preventive handling precautions

Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation. For precautions see section 2.2.

#### General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

### 7.2. Conditions for safe storage, including any incompatibilities

Store at ambient temperature. Store in a dry place. Store in a closed container.

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### Exposure limits

No occupational exposure limit assigned.

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## 8.2. Exposure controls

### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

#### Hand protection

Wear protective gloves.

Breakthrough time:

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals.

Wash contaminated skin thoroughly after handling.

#### Other skin protection

Wash skin thoroughly after handling.

#### Respiratory protection

Provide adequate ventilation.

#### Environmental exposure controls

Avoid discharge into drains.

## SECTION 9: Physical and chemical properties

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

#### Physical state

Liquid

#### Colour

Colourless.

#### Odour

No data available

#### Melting point / freezing point

-38 °C

#### Boiling point or initial boiling point and boiling range

71 - 72 °C

#### Flammability

No data available

#### Lower and upper explosion limit

0.1 - 1.1 %

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## Flash point

66 °C

## Auto-ignition temperature

No data available

## Decomposition temperature

No data available

## pH

5.7

## Kinematic viscosity

No data available

## Solubility

8.6 g/l

## Partition coefficient n-octanol/water

0.67

## Vapour pressure

No data available

## Density and/or relative density

0.954

## Relative vapour density

No data available

## Particle characteristics

No data available

## 9.2. Other information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Forms explosive mixtures with air on intense heating.

15 (approx) Kelvin below the flash point is to be rated as critical.

### 10.2. Chemical stability

Stable under the prescribed storage conditions.

### 10.3. Possibility of hazardous reactions

No data available

### 10.4. Conditions to avoid

strong heating

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## 10.5. Incompatible materials

Strong oxidising agents. Strong bases

## 10.6. Hazardous decomposition products

See section 5.

## SECTION 11: Toxicological information

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

#### Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Duration of exposure	Test animals
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	LD50	>2000 mg/kg	Oral	-	Rat
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	LC50	>73 mg/l	Inhalation.	6 hours	Rat

#### Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Species
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	Causes mild skin irritation.	Rabbit

#### Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Species
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	No eye irritation.	Rabbit

#### Germ cell mutagenicity

Product / Substance name CAS / EC no.	Result	Species	Method / Guideline
tert-Butyl acetoacetate	Negative.	S. typhimurium	Ames test

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Product / Substance name CAS / EC no.	Result	Species	Method / Guideline
1694-31-1 / 216-904-5			

## Aspiration hazard

Based on available data, the classification criteria are not met.

## 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

#### Acute fish toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	LC50	320 mg/l	96 hours	Pimephales promelas (Fat-head Minnow)

#### Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
tert-Butyl acetoacetate 1694-31-1 / 216-904-5	EC50	320 mg/l	48 hours	Daphnia magna

### 12.2. Persistence and degradability

No data available

### 12.3. Bioaccumulative potential

No data available

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

No data available

### 12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.



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## 12.7. Other adverse effects

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

## SECTION 14: Transport information

### 14.1. UN number

Not applicable

### 14.2. UN proper shipping name

Not applicable

### 14.3. Transport hazard class(es)

Not applicable

### 14.4. Packing group

Not applicable

### 14.5. Environmental hazards

Not applicable

### 14.6. Special precautions for user

Not applicable

### 14.7. Maritime transport in bulk according to IMO instruments

Not applicable

## SECTION 15: Regulatory information

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

#### EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

#### National regulations

Regulation 2019/1148: Acetone.

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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## SECTION 16: Other information

No data available