

## Chemical Safety Data Sheet MSDS / SDS

**tert-Butyl acetoacetate**Revision Date:2024-12-21 Revision Number:1

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

Product name : tert-Butyl acetoacetate  
CBnumber : CB0441030  
CAS : 1694-31-1  
EINECS Number : 216-904-5  
Synonyms : TBAA,tert-butyl acetoacetate

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Signal word : Warning

**Precautionary statements**

P501 Dispose of contents/container to....  
P403+P235 Store in a well-ventilated place. Keep cool.  
P370+P378 In case of fire: Use ... for extinction.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

**Hazard statements**

H227 Combustible liquid

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**SECTION 3: Composition/information on ingredients****Substance**

Product name	: tert-Butyl acetoacetate
Synonyms	: TBAA,tert-butyl acetoacetate
CAS	: 1694-31-1
EC number	: 216-904-5
MF	: C8H14O3
MW	: 158.2

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### Unsuitable extinguishing media

Do NOT use water jet.

### Special hazards arising from the substance or mixture

Carbon oxides

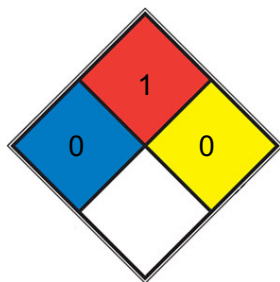
### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

## NFPA 704



HEALTH 0 Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

SPEC.

HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

## Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance colourless clear, liquid

Odour No data available

Odour Threshold No data available

pH 5,7 at 9 g/l at 20 °C

Melting point/freezing point	Melting point/range: -31,5 °C
Initial boiling point and boiling range	71 - 72 °C at 15 hPa
Flash point	66 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 1,1 %(V) Lower explosion limit: 0,1 %(V)
Vapour pressure	No data available
Vapour density	No data available
Relative density	0,954 g/mL at 25 °C
Water solubility	8,6 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 0,67
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

Heat, flames and sparks.

### Incompatible materials

Strong acids, Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - > 2.000 mg/kg

LC50 Inhalation - Rat - 6 h - > 73 mg/l

#### Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

Ames test

S. typhimurium Result: negative

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### Reproductive toxicity

No data available

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

No data available

#### Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

### Toxicity

#### Toxicity to fish

LC50 - Pimephales promelas (fathead minnow) - 320 mg/l - 96 h

#### Toxicity to daphnia and other aquatic invertebrates

Immobilization EC50 - Daphnia magna (Water flea) - 320 mg/l - 48 h

#### Persistence and degradability

No data available

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

### **Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### **Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### **Waste treatment methods**

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### **Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### **UN number**

ADR/RID: - IMDG: - IATA: -

### **UN proper shipping name**

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

### **Transport hazard class(es)**

ADR/RID: - IMDG: - IATA: -

### **Packaging group**

ADR/RID: - IMDG: - IATA: -

### **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no IATA: no

### **Special precautions for user**

No data available

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## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

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## SECTION 16: Other information

### Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

### References

**[1]** CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

**[2]** ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

**[3]** ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**[4]** eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

**[5]** ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

**[6]** Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

**[7]** HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

**[8]** IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

**[9]** IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

**[10]** Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>



**Disclaimer:**

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