

## SAFETY DATA SHEET

Version 6.5  
Revision Date 04/28/2022  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : *tert*-Butyl acetoacetate

Product Number : 688770  
Brand : Aldrich  
CAS-No. : 1694-31-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 4), H227

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram none

Signal Word Warning

Hazard statement(s)  
H227 Combustible liquid.

Precautionary statement(s)  
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No  
smoking.

|             |                                                                                       |
|-------------|---------------------------------------------------------------------------------------|
| P280        | Wear protective gloves/ protective clothing/ eye protection/ face protection.         |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction. |
| P403 + P235 | Store in a well-ventilated place. Keep cool.                                          |
| P501        | Dispose of contents/ container to an approved waste disposal plant.                   |

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                 |
|------------------|-------------------------------------------------|
| Formula          | : C <sub>8</sub> H <sub>14</sub> O <sub>3</sub> |
| Molecular weight | : 158.19 g/mol                                  |
| CAS-No.          | : 1694-31-1                                     |

| Component                      | Classification     | Concentration |
|--------------------------------|--------------------|---------------|
| <b>tert-Butyl acetoacetate</b> |                    |               |
|                                | Flam. Liq. 4; H227 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### 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.

### 4.2 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

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

No data available

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## **SECTION 5: Firefighting measures**

### **5.1 Extinguishing media**

#### **Suitable extinguishing media**

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

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

Carbon oxides

### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

### **5.4 Further information**

Use water spray to cool unopened containers.

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## **SECTION 6: Accidental release measures**

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

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas. For personal protection see section 8.

### **6.2 Environmental precautions**

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

### **6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Avoid inhalation of vapor or mist.

#### **Advice on protection against fire and explosion**

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

#### **Hygiene measures**

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

For precautions see section 2.2.

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

#### **Storage conditions**

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

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### 7.3 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

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Hazardous components without workplace control parameters

### 8.2 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.

##### 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

### 9.1 Information on basic physical and chemical properties

- |                   |                                  |
|-------------------|----------------------------------|
| a) Appearance     | Form: liquid<br>Color: colorless |
| b) Odor           | No data available                |
| c) Odor Threshold | No data available                |
| d) pH             | 5.7 at 9 g/l at 20 °C (68 °F)    |

|                                                 |                                                                    |
|-------------------------------------------------|--------------------------------------------------------------------|
| e) Melting point/freezing point                 | Melting point/range: -38 °C (-36 °F)                               |
| f) Initial boiling point and boiling range      | 71 - 72 °C 160 - 162 °F at 15 hPa                                  |
| g) Flash point                                  | 66 °C (151 °F) - closed cup                                        |
| h) Evaporation rate                             | No data available                                                  |
| i) Flammability (solid, gas)                    | No data available                                                  |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 1.1 %(V)<br>Lower explosion limit: 0.1 %(V) |
| k) Vapor pressure                               | No data available                                                  |
| l) Vapor density                                | No data available                                                  |
| m) Density                                      | 0.954 g/mL at 25 °C (77 °F)                                        |
| Relative density                                | No data available                                                  |
| n) Water solubility                             | 8.6 g/l at 20 °C (68 °F)                                           |
| o) Partition coefficient: n-octanol/water       | log Pow: 0.67                                                      |
| p) Autoignition temperature                     | No data available                                                  |
| q) Decomposition temperature                    | No data available                                                  |
| r) Viscosity                                    | No data available                                                  |
| s) Explosive properties                         | No data available                                                  |
| t) Oxidizing properties                         | No data available                                                  |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg

(Calculation method)

LD50 Oral - Rat - > 2,000 mg/kg

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

Dermal: No data available

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

#### Carcinogenicity

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

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### Reproductive toxicity

No data available

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

### 11.2 Additional Information

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

### 12.1 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 |

### 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

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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

### DOT (US)

NA-Number: 1993    Class: NONE    Packing group: III  
Proper shipping name: Combustible liquid, n.o.s. (tert-Butyl acetoacetate)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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## SECTION 15: Regulatory information

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Fire Hazard

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

|                         | CAS-No.   | Revision Date |
|-------------------------|-----------|---------------|
| tert-Butyl acetoacetate | 1694-31-1 |               |
| acetone                 | 67-64-1   | 1993-02-16    |
| tert-Butanol            | 75-65-0   | 2007-03-01    |

### New Jersey Right To Know Components

|                         | CAS-No.   | Revision Date |
|-------------------------|-----------|---------------|
| tert-Butyl acetoacetate | 1694-31-1 |               |

### California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

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## SECTION 16: Other information

### Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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