

## SAFETY DATA SHEET

Version 4.12  
Revision Date 02/14/2018  
Print Date 10/19/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : *tert*-Butyl acetoacetate

Product Number : 537594  
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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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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 P280 P370 + P378	Keep away from heat/sparks/open flames/hot surfaces. No smoking. Wear protective gloves/ eye protection/ face protection. In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P235 P501	Store in a well-ventilated place. Keep cool. Dispose of contents/ container to an approved waste disposal plant.

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

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3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Synonyms : TBAA

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

#### Hazardous components

Component	Classification	Concentration
<b>tert-Butyl acetoacetate</b>	Flam. Liq. 4; H227	90 - 100 %

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

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## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this 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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## 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

No data available

### 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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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 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.

### 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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## 7. HANDLING AND STORAGE

### 7.1 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.

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

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

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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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components 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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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                    |   |
|--------------------|---|
| a) Appearance      | Form: clear, liquid<br>Colour: colourless |
| b) Odour           | No data available                         |
| c) Odour 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: -31.49 °C (-24.68 °F)
f) Initial boiling point and boiling range	71 - 72 °C (160 - 162 °F) at 15 hPa (11 mmHg)
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) Lower explosion limit: 0.1 %(V)
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	0.954 g/mL at 25 °C (77 °F)
n) Water solubility	8.6 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: 0.67
p) Auto-ignition 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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## 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

Strong acids, Strong oxidizing agents

### 10.6 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

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

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 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.

NTP: No component 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

**Additional Information**

RTECS: Not available

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

Kidney - Irregularities - Based on Human Evidence (Acetone)

Skin - Dermatitis - Based on Human Evidence (Acetone)

Liver - Irregularities - Based on Human Evidence (tert-Butyl alcohol)

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## 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 Other adverse effects

No data available

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## 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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## 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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## 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-Butyl alcohol	75-65-0	2007-07-01

### 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 State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

Flam. Liq. H227	Flammable liquids Combustible liquid.
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**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

**NFPA Rating**

Health hazard:	0
Fire Hazard:	2
Reactivity Hazard:	0

**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.

**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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