

SAFETY DATA SHEET

1. PRODUCT

1.1 Product identifiers

Name: tert-Butyl acetoacetate

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

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	N/A
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

No data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula: $C_8H_{14}O_3$
Molecular weight: 158.19 g/mol
CAS-No.: 1694-31-1

Hazardous components

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

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

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

4.2 Indication of any immediate medical attention and special treatment needed

No data available

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.

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.

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.

Recommended storage temperature -20 °C

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Hazardous components without workplace 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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

Appearance	Form: clear, liquid Colour: colourless
Odour	No data available
Odour Threshold	No data available
pH	5.7 at 9 g/l at 20 °C (68 °F)
Melting point/freezing point	Melting point/range: -31.5 °C (-24.7 °F)
Initial boiling point and boiling range	71 - 72 °C (160 - 162 °F) at 15 hPa (11 mmHg)
Flash point	66 °C (151 °F) - 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 (77 °F)
Water solubility	8.6 g/l at 20 °C (68 °F)

Partition coefficient: n-octanol/water	log Pow: 0.67
Auto-ignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

9.2 Other safety information

No data available

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

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 identified as a carcinogen or potential carcinogen by OSHA.
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)

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
Toxicity to algae	No data available
Toxicity to bacteria	No data available

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

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.

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

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

Component	CAS-No.	Revision Date
tert-Butyl acetoacetate	1694-31-1	
Acetone	67-64-1	2007-03-01
tert-Butyl alcohol	75-65-0	2007-07-01

New Jersey Right To Know Components

Component	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.

16. OTHER INFORMATION**Full text of H-Statements referred to under sections 2 and 3.**

Flam. Liq. Flammable liquids

H227 Combustible liquid.

HMIS Rating

Health hazard: 2

Chronic Health Hazard: *

Flammability: 2

Physical Hazard 0

NFPA Rating

Health hazard: 0

Fire Hazard: 2

Reactivity Hazard: 0
