

SAFETY DATA SHEET

Revision Date 26-Mar-2024

Revision Number 4

1. Identification

Product Name tert-Butyl acetoacetate
Cat No. : A11115
CAS No 1694-31-1
Synonyms No information available
Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids

Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Combustible liquid

Precautionary Statements

Prevention

Keep away from heat/sparks/open flames/hot surfaces. - No smoking

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

Fire

In case of fire: Use CO₂, dry chemical, or foam for extinction

Storage

Store in a well-ventilated place. Keep cool

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

| Component | CAS No | Weight % |
|--|-----------|----------|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | 99 |

4. First-aid measures

| | |
|--|--|
| Eye Contact | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention. |
| Skin Contact | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention. |
| Ingestion | Do NOT induce vomiting. Clean mouth with water. Get medical attention. |
| Most important symptoms and effects | Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting |
| Notes to Physician | Treat symptomatically |

5. Fire-fighting measures

| | |
|---|--|
| Suitable Extinguishing Media | Water spray. Carbon dioxide (CO ₂). Dry chemical. Water mist may be used to cool closed containers. Chemical foam. Water mist may be used to cool closed containers. |
| Unsuitable Extinguishing Media | No information available |
| Flash Point | 76 °C / 168.8 °F |
| Method - | No information available |
| Autoignition Temperature | 390 °C / 734 °F |
| Explosion Limits | |
| Upper | .00% |
| Lower | 1.10% |
| Sensitivity to Mechanical Impact | No information available |
| Sensitivity to Static Discharge | No information available |

Specific Hazards Arising from the Chemical

Combustible material. Flammable. Containers may explode when heated.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

| | | | |
|---------------|---------------------|--------------------|-------------------------|
| Health | Flammability | Instability | Physical hazards |
| 0 | 1 | 0 | N/A |

6. Accidental release measures

| | |
|---|--|
| Personal Precautions | Remove all sources of ignition. Take precautionary measures against static discharges. |
| Environmental Precautions | See Section 12 for additional Ecological Information. |
| Methods for Containment and Clean Up | Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. |

7. Handling and storage

| | |
|-----------------|--|
| Handling | Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Take precautionary measures against static discharges. Keep away from open flames, hot surfaces and sources of ignition. |
| Storage. | Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Strong oxidizing agents. Strong bases. |

8. Exposure controls / personal protection

| | |
|--------------------------------------|---|
| Exposure Guidelines | This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies. |
| Engineering Measures | None under normal use conditions. Ensure adequate ventilation, especially in confined areas. |
| Personal Protective Equipment | |
| Eye/face Protection | Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166. |
| Skin and body protection | Wear appropriate protective gloves and clothing to prevent skin exposure. |
| Respiratory Protection | No protective equipment is needed under normal use conditions. |
| Recommended Filter type: | Particle filter. |
| Hygiene Measures | Handle in accordance with good industrial hygiene and safety practice. |

9. Physical and chemical properties

| | |
|----------------------------|----------------------------|
| Physical State | Liquid |
| Appearance | Yellow |
| Odor | Odorless |
| Odor Threshold | No information available |
| pH | No information available |
| Melting Point/Range | -38 °C / -36.4 °F |
| Boiling Point/Range | 190 °C / 374 °F @ 760 mmHg |
| Flash Point | 76 °C / 168.8 °F |
| Evaporation Rate | No information available |

| | |
|---|--------------------------|
| Flammability (solid,gas) | Not applicable |
| Flammability or explosive limits | |
| Upper | .00% |
| Lower | 1.10% |
| Vapor Pressure | No information available |
| Vapor Density | 5.5 |
| Specific Gravity | 0.970 |
| Solubility | No information available |
| Partition coefficient; n-octanol/water | No data available |
| Autoignition Temperature | 390 °C / 734 °F |
| Decomposition Temperature | No information available |
| Viscosity | No information available |
| Molecular Formula | C8 H14 O3 |
| Molecular Weight | 158.2 |

10. Stability and reactivity

| | |
|---|--|
| Reactive Hazard | None known, based on information available |
| Stability | Stable. |
| Conditions to Avoid | Exposure to air. Exposure to light. Incompatible products. Keep away from open flames, hot surfaces and sources of ignition. |
| Incompatible Materials | Strong oxidizing agents, Strong bases |
| Hazardous Decomposition Products | Carbon monoxide (CO), Carbon dioxide (CO ₂) |
| Hazardous Polymerization | Hazardous polymerization does not occur. |
| Hazardous Reactions | None under normal processing. |

11. Toxicological information

Acute Toxicity

Product Information No acute toxicity information is available for this product

Component Information

Toxicologically Synergistic No information available

Products

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

| Component | CAS No | IARC | NTP | ACGIH | OSHA | Mexico |
|--|-----------|------------|------------|------------|------------|------------|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | Not listed | Not listed | Not listed | Not listed | Not listed |

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT COMBUSTIBLE LIQUID, NOT REGULATED FOR TRANSPORT IN THIS QUANTITY
According to 49 CFR §173.150(f)(1), this material should be reclassified as NA1993, Combustible Liquid, NOS if it is shipped in bulk.

UN-No NA1993
Proper Shipping Name Combustible liquid, n.o.s.
Packing Group III

TDG Not regulated
IATA Not regulated
IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | TSCA - EPA Regulatory Flags |
|--|-----------|------|---|-----------------------------|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | X | ACTIVE | PMN |

Legend:
TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)
 X - Listed
 - - Not Listed
 PMN - Indicates a commenced PMN substance

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

| Component | CAS No | DSL | NDSL | EINECS | PICCS | ENCS | ISHL | AICS | IECSC | KECL |
|--|-----------|-----|------|-----------|-------|------|------|------|-------|---------|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | X | - | 216-904-5 | X | X | X | X | X | 97-3-83 |

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|--|-----------|---|---|---|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | - | - | - |

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

| Component | CAS No | OECD HPV | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|--|-----------|----------------|------------------------------|---------------------------|--|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | Not applicable | Not applicable | Not applicable | Not applicable |

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|--|-----------|---|--|----------------------------|------------------------------------|
| Butanoic acid, 3-oxo-, 1,1-dimethylethyl ester | 1694-31-1 | Not applicable | Not applicable | Not applicable | Not applicable |

16. Other information

Prepared By

Health, Safety and Environmental Department
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 www.thermofisher.com

Revision Date

26-Mar-2024

Print Date

26-Mar-2024

Revision Summary

New emergency telephone response service provider.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS