



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

Date of Compilation : March 30, 2021
Date of Revision : April 01, 2024
Revision due date : March 2027
Revision Number : 02
Version Name : 1078Gj Ghs02 Div.03 sds Tert. Butyl Acetoacetate
Supersedes date : October 08, 2021
Supersedes version : 1078Gj Ghs01 Div.03 sds Tert. Butyl Acetoacetate

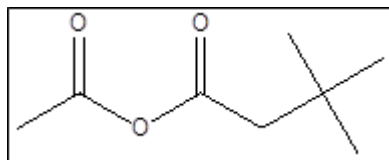
Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/ UNDERTAKING

1.1 Product Identifier

Product name	: Tert. Butyl Acetoacetate
CAS RN	: 1694-31-1
EC#	: 216-904-5
Synonyms	: Acetoacetic acid, tert-butyl ester; 3-Oxobutyric acid tert-butyl ester; tert-Butyl 3-oxobutyrate; tert-Butyl acetylacetate; tert-Butyl acetylacetonate; tert-butyl 3-oxobutanoate; 3-Oxobutanoic acid 1,1-dimethylethyl ester, 1,1-Dimethylethyl acetoacetate
Technical name	: tert-butyl 3-oxobutanoate
Molecular formula	: C ₈ H ₁₄ O ₃
Structural formula	:



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

Relevant identified uses: Raw material in pharmaceutical Industry, In Agrochemical industry; Reagent for Acyloin synthesis and alpha, beta unsaturated ketones synthesis

Uses advised against: None

1.3. Details of the supplier of the safety data sheet

Jubilant Ingrevia Limited

FACTORY & REGISTERED OFFICE:

Jubilant Ingrevia Limited., Bhartiagram, Gajraula, District: Amroha, Uttar Pradesh-244223, India
T +91-5924-267437& +91-5924-267438

HEAD OFFICE: Jubilant Ingrevia Limited., Plot 1-A, Sector 16-A, Institutional Area, Noida, Uttar Pradesh, 201301 – India T +91-120-4361000 - F +91-120-4234881 / 84 / 85 / 87 / 95 / 96 support@jubl.com - www.jubilantingrevia.com

1.4. Emergency telephone number

For Chemical Emergency ONLY (in the case of fire, leak, spill, exposure or accident) Call
Chemtrec: 1-800-424-9300 (US), 1-703-527-3887 (Outside U.S.)
Chemtrec (India) : 000-800-100-7141

For ALL other emergencies call Emergency Control Room Gajraula at 99970 22412

SECTION 2: HAZARD(S) IDENTIFICATION



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

2.1 Classification of the substance or mixture

GHS-US classification

Flammable liquids Category 4

2.2 Label Elements

Pictograms: None

Signal word: Warning!

Hazard and Precautionary Statements:

HAZARD STATEMENTS

H227: Combustible liquid.

PRECAUTIONARY STATEMENTS

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

P403+P235: Store in a well-ventilated place. Keep cool.

P501: Dispose of contents/container to local/regional/national/international regulations.

2.3 Other Hazards

Not known.

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Substance	CAS Number	EC Number	Assay/Purity
Tert. Butyl Acetoacetate	1694-31-1	216-904-5	NLT 98.0%

3.2 Mixtures

- Not applicable.

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.

4.2. Most important symptoms and effects, both acute and delayed:

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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

Treatment: Treat symptomatically.

SECTION 5: FIRE-FIGHTING MEASURES

5.1 : Extinguishing media

Suitable extinguishing media: CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

5.2 : Special hazards arising from the substance or mixture

Specific hazards during fire fighting : Combustible material. Flammable. Containers may explode when heated

Hazardous Combustion Products: Carbon monoxide (CO). Carbon dioxide (CO₂).

5.3 : Advice for firefighters

Special fire fighting procedures: Fight fire from a protected location. Use water spray to cool unopened containers.

Special protective equipment for fire-fighters: Wear an approved positive pressure self-contained breathing apparatus in addition to standard fire fighting gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1 : Personal precautions, protective equipment and emergency procedures

Personal precautions: Personal precautions: Wear appropriate personal protective equipment. Local authorities should be advised if significant spillages cannot be contained.

6.2 : Environmental precautions

Prevent further leakage or spillage if safe to do so. Use appropriate container to avoid environmental contamination. Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained. If the product contaminates rivers and lakes or drains inform respective authorities.

6.3 : Methods and materials for containment and cleaning up

Methods for cleaning 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

6.4 : Reference to other sections

Never return spills in original containers for re-use. Dispose of in accordance with local regulations.

SECTION 7: HANDLING AND STORAGE

7.1 : Precautions for safe handling

Safe Handling:

- Wash hands before breaks and immediately after handling the product.
- Remove and wash contaminated clothing before re-use.
- Use only clean equipment.
- Wear personal protective equipment. For personal protection see section 8.
- Provide appropriate exhaust ventilation.
- Take measures to prevent the build up of electrostatic charge.
- Keep away from fire (No Smoking). Keep away from fire, sparks and heated surfaces.
- Do not use sparking tools.
- Do not breathe mist or vapor.
- Do not get in eyes, on skin, on clothing.



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

- Do not taste or swallow.

7.2 : Storage

- Keep upright in properly labelled containers.
- Containers which are opened must be carefully resealed and kept upright to prevent leakage
- Keep containers tightly closed in a dry and well-ventilated place away from incompatible materials.
- Keep away from moisture.

7.3 : Specific end use(s)

- Not available

SECTION 8: EXPOSURE CONTROLS / PERSONAL PROTECTION

8.1 : Control parameters

- Country specific exposure limits have not been established or are not applicable unless listed below.

: Exposure Limits Values

- No Information available

: Exposure Limits (International)

- No Information available

: Derived No-Effect-Levels (DNEL) Predicted No-Effect-concentration (PNEC)

- No Information available

8.2 : Exposure controls

General protective and hygiene measures

- Wear protective gloves/protective clothing/eye protection/face protection.
- The standard precautionary measures should be adhered to when handling
- Wash hands during breaks and at the end of handling the material
- Immediately remove any contaminated clothing

Appropriate Engineering Controls:

- Good general ventilation (typically 10 air changes per hour) should be sufficient to control airborne levels. Ensure adequate ventilation. If applicable, use process enclosures, local exhaust ventilation, or other engineering controls to maintain airborne levels below recommended exposure limits. If exposure limits have not been established, maintain airborne levels to an acceptable level.

: Personal Protection

Eyes: Based on an evaluation of the eye or face hazards present, wear chemical splash-resistant safety glasses or goggles with side protection. A face shield may be appropriate in some workplaces. Use eyewear tested and approved under appropriate government standards such as OSHA 29 CFR 1910.133 or EU EN166.

Hands: Wear gloves selected based on an evaluation of the possible hazards to hands and skin, the duration of use, the physical conditions of the workplace, and the chemical resistance and physical properties of the glove material.

Skin and body: Protective clothing must be selected based on the hazards present in the workplace, the physical environment, the duration of exposure, and other factors. No fabric can provide protection against all

Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

potential hazards; therefore it is important to select the appropriate protective clothing for each specific hazard. At the minimum, wear a laboratory coat and close-toed footwear.

Respiratory: Where risk assessment shows air-purifying respirators are appropriate use a dust mask type N95 (US) or type P1 (EN 143) respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Respirator type: Air purifying respirator with an appropriate, government approved (where applicable), air-purifying filter, cartridge or canister. Contact health and safety professional or manufacturer for specific information.

: Occupational hygiene

- No data available.

: Additional Information

- No data available.

: Control of environmental exposure

- Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1 : Information on basic physical and chemical properties.

Sr. No.	Parameter	Typical value
1.	Appearance	Clear colorless to light yellow liquid
2.	Molecular weight	158.19
3.	Odor	Odourless
4.	Odor Threshold	No information available
5.	pH	5.7 at 9 g/l at 20 °C
6.	Melting/freezing point	(-)38 °C
7.	Boiling point	174°C
8.	Flash point	60.56 °C
9.	Evaporation rate (n-BuAc=1)	Not determined
10.	Flammability (solid/gas)	Non applicable
11.	Upper/lower flammability or Explosive limits	Upper explosion limit: 1.1 %(V) Lower explosion limit: 0.1 %(V)
12.	Vapor pressure	0.749 Torr Temp: 25 °C
13.	Vapour density (air=1)	Not determined
14.	Density	0,954 g/mL at 20 °C
15.	Solubility	8.6 g/l at 20 °C in water and soluble in Xylene.
16.	Partition coefficient (Octonol /water)	1.41± 0.33
17.	Auto-ignition temperature	390 °C (734 °F)
18.	Decomposition temperature	195°C (624°F)
19.	Viscosity	12.75 mPa s (dynamic) at 32 deg C
20.	Explosive property	Non-Explosive

Tert. Butyl Acetoacetate
Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

Sr. No.	Parameter	Typical value
21.	Oxidizing property	Oxidising material

9.2 : Other information

- Not available

SECTION 10: STABILITY AND REACTIVITY

- 10.1 Reactivity:** None known, based on information available
- 10.2 Chemical stability:** Stable under normal storage conditions.
- 10.3 Possibility of hazardous reactions:** None.
- 10.4 Conditions to avoid:** Exposure to air. Exposure to light. Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
- 10.5 Incompatible materials:** Strong oxidizing agents, Strong bases
- 10.6 Hazardous decomposition Products :** Carbon monoxide, Carbon dioxide.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1 : Information on toxicological effects

Acute Toxicity:

Oral LD-50: (Rat): 4100 mg/kg bw in males;4750 mg/kg bw in females and 4500 mg/kg bw in both sex,when male and female wistar albino rats

Skin irritation/corrosion : Not Irritating

Species : Rabbit

Eye damage/irritation: Not Irritating

Species : Rabbit eye

Respiratory or skin sensitization: Not sensitizing

Germ cell mutagenicity: Not classified based on available information.

Carcinogenicity: This product does not contain any carcinogens or potential carcinogens as listed by OSHA, IARC or NTP.

Reproductive toxicity: Not classified based on available information.

Remarks: No data available.

Specific target organ system toxicity - repeated exposure: Not classified based on available information.

Remarks: No data available.

Specific target organ system toxicity - single exposure: Not classified based on available information.

Remarks: No data available.

Aspiration hazard: No aspiration toxicity classification.

Additional information:

The toxicological data given are determined by analogy.

Symptoms / effects,both acute and delayed

Immediate effects

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

RTECS: Not available

SECTION 12: ECOLOGICAL INFORMATION

12.1 : Toxicity

- Short-term toxicity to aquatic invertebrates
LC50: 2 042 mg/L
- Toxicity to aquatic algae and cyanobacteria
EC50 for freshwater algae: 459 mg/L

12.2 : Persistence and degradability

Tert. Butyl Acetoacetate	
Persistence and degradability	Readily biodegradable Soluble in water Persistence is unlikely based on information available.

12.3 : Bio accumulative potential

Tert. Butyl Acetoacetate	
Bio accumulative potential	3.162 L/kg ww
Log Kow	1.41± 0.33

12.4 : Mobility in Soil

Tert. Butyl Acetoacetate	
Soil Adsorp. Coeff. (Estimated Koc)	Koc at 20 °C: 10
Henry's Law Constant	Not available

12.5 : Other adverse effects

- Results of PBT and vPvB assessment: Not fulfilling vPvB (very persistent, very bioaccumulative) criteria.

SECTION 13: DISPOSAL CONSIDERATIONS

13.1 : Disposal of waste

- **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.

SECTION 14: TRANSPORT INFORMATION

- This substance is considered to be non-Hazardous for transport by Air/ Rail/ Road and Sea and thus not regulated by IATA/ ICAO/ US DOT/ IMO/ IMDG.

	ADR/ RID/ DOT	IMDG	IATA
14.1 UN number	--	--	--
14.2 UN proper shipping name			



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

Not a Dangerous Good	Not a Dangerous Good	Not Dangerous Good
14.3 Transport hazard class(es)		
--	--	--
14.4 Packing group		
--	--	--
14.5 Environmental hazards		
No	No	No

14.6 Special instructions for user.

- The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations

14.7. Transport in bulk according to Annex II of Marpol and IBC code

- Not available

SECTION 15: REGULATORY INFORMATION

Classification as per CLP Regulation 1272/2008:

Not Classified

Hazard Statements:

None

Chemical Inventory Lists:	Status
TSCA:	Listed
EC Inventory	216-904-5
Canada(DSL/NDSL):	Listed (DSL)
Taiwan Chemical Substance Inventory (TCSI)	Listed
New Zealand Inventory of Chemicals (NZIoC)	Listed
Philippines Inventory of Chemicals and Chemical Substances (PICCS)	Listed
Inventory of Existing and New Chemical Substances (ENCS)	Listed
Japan ISHL Existing Substances List (ISHL)	Not Listed
China: IECSC	Listed
Catalog of Hazardous chemical(2015) China	Not Listed
Existing Chemicals List (KECI)	Listed
Australian Inventory of Chemical Substances (AICS)	Listed

SECTION 16: OTHER INFORMATION

a) : Compilation information of safety data sheet

Date of Compilation : March 30, 2021
 Date of Revision : April 01, 2024
 Revision due date : March, 2027
 Revision Number : 02
 Version Name : 1078Gj Ghs02 Div.03 sds Tert. Butyl Acetoacetate
 Supersedes date : October 08, 2021



Tert. Butyl Acetoacetate Safety Data Sheet

According to the federal final rule of hazard communication revised on 2012 (HazCom 2012)

Supersedes version : 1078Gj Ghs01 Div.07 sds Tert. Butyl Acetoacetate

b) A key or legend to aberrations and acronyms used in the safety data sheet

SCBA	= Self Contained Breathing Apparatus.
NIOSH REL	= National Institute for Occupational Safety and Health Recommended Exposure Limit.
OSHA PEL	= Occupational Safety and Health Administration Permissible Exposure Limit.
RTECS	= Registry of Toxic Effects of Chemical Substances.
IARC	= International Agency for Research on Cancer.
TSCA	= Toxic Substances Control Act.
DSL/NDL	= Domestic/Non-Domestic Substances List.
TLV	= Threshold Limit Value.
ACGIH	= American Conference of Governmental Industrial Hygienists.
REACH	= Registration, Evaluation, Authorization and Restriction of Chemicals.
CLP	= Classification, Labeling and Packaging.
GHS	= Globally Harmonized System.
IMDG-Code	= International Maritime Code for Dangerous Goods.
ICAO	= International Civil Aviation Organization.
IATA/DGR	= International Air Transport Association/Dangerous Goods Regulation.

c) Key Literature reference and sources for data

Biographical reference and data sources

- Globally Harmonized System of Classification and Labelling of Chemicals.
- CLP REG (regulation) (EC) no. 1272/2008, last modification by regulation (EC) no. 790/2009
- REG (EC) no. 1907/2006, last modification by REG (EC) Nr. 830/2015

d) List of hazard statements

Hazards Statements	H227: Combustible liquid.
---------------------------	---------------------------

SDS US (GHS HazCom 2012)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.

(End of Safety Data Sheet)