**tert-Butyl acetoacetate**  
(TBAAE, TBAA)

**CAS No.** 1694-31-1  
**HS Code** 2918 30 90  
**EINECS No.** 216-904-5

**Synonyms**  
tert-Butyl-3-ketobutrate; tert-Butyl acetylacetate  
1',1'-Dimethylethyl-3-ketobutrate; 1',1'-Dimethylethyl acetylacetate; tert-Butyl acetone carboxylate  
tert-Butyl-3-oxo butanoate; 1,1-Dimethylethyl acetone carboxylate; 1',1'-Dimethylethyl-3-oxo butanoate; Acetoacetic acid tert-Butyl ester  
Acetoacetic tert-Butyl ester

**Molecular Formula** C₈H₁₄O₃

**Chemical Structure**

```
H₃C
O
H₃C
O
H₃C
CH₃
```

**Molecular Weight** 158

**Quality**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Colour</strong></td>
<td>Colourless to slightly yellow</td>
</tr>
<tr>
<td><strong>Consistency</strong></td>
<td>Clear Liquid</td>
</tr>
<tr>
<td><strong>Moisture Content %, max</strong></td>
<td>0.2</td>
</tr>
<tr>
<td><strong>Acidity (as Acetic acid) %, max</strong></td>
<td>0.2</td>
</tr>
<tr>
<td><strong>Purity (by GC) %, min</strong></td>
<td>99</td>
</tr>
<tr>
<td><strong>Colour value APHA, max</strong></td>
<td>50</td>
</tr>
</tbody>
</table>

**Packaging**

- Bulk Tankers, 200kg HMHDPE Drums, IBCs  
- ISO Tanks

**Application**

- Raw material in pharmaceutical Industry  
- In Agrochemical industry; Reagent for Acyloin synthesis and α,β – unsaturated ketones synthesis

**Country of Origin**

India

*For further information please visit [www.laxmiorganic.co.in](http://www.laxmiorganic.co.in) or send an enquiry to info@laxmiorganic.co.in*
01 Identification of the substance/mixture and of the company/undertaking

Product details: Tertiary butyl acetoacetate

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

Application of the substance / the preparation
An important synthetic raw material, used as pharmaceutical intermediates.

02 Hazards Identification

Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008:
The substance is not classified as Hazardous according to the CLP regulation.

Classification according to Directive 67/548/EEC or Directive 1999/45/EC
Not applicable

Information concerning particular hazards for human and environment: Not applicable
Label elements

Labelling according to Regulation (EC) No 1272/2008
The substance is classified and labelled according to the CLP regulation.

Hazard pictograms  
Signal word  
Hazard-determining components of labelling: Void  
Hazard statements  

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.
vPvB: Not applicable.

03 Composition/Information on Ingredients

Chemical characterization:

CAS No.: 1694-31-1  Description: Tertiary butyl acetoacetate

Identification number(s)  
EINECS Number : 216-904-5  

Additional information:
Molecular formula : C8H14O3  
Molecular Weight : 158.195
04 First Aid Measures

After inhalation:
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

After skin contact:
Immediately wash with water and soap and rinse thoroughly. Seek medical treatment.

After eye contact:
Rinse opened eye for several minutes under running water.

After swallowing:
If symptoms persist consult doctor.

Information for doctor:
Most important symptoms and effects, both acute and delayed:
No further relevant information available.

Indication of any immediate medical attention and special treatment needed:
No further relevant information available.

05 Firefighting Measures

Extinguishing media:

Suitable extinguishing agents:
In case of fire, use sand, carbon dioxide or powdered extinguishing media.

For safety reasons unsuitable extinguishing agents:
Water

Advice for firefighters

Protective equipment:
Wear self contained breathing apparatus.
Wear fully protective suit.

Personal precautions, protective equipment and emergency procedures:
Wear protective equipment. Keep unprotected persons away. Ensure adequate ventilation.

Environmental precautions:
Do not allow product to reach sewage system or any water course.

Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). Dispose of the material collected according to regulations.

Reference to other sections:
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

06 Accidental Release Measures

Personal precautions, protective equipment and emergency procedures:
Wear protective equipment. Keep unprotected persons away. Ensure adequate ventilation.

Environment precautions:
Do not allow product to reach sewage system or any water course.

Methods and material for containment and cleaning up:
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). Dispose of the material collected according to regulations.

Reference to other sections:
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.
Handling and Storage

Handling

Precautions for safe handling:
Store in cool, dry place in tightly closed receptacles.
Ensure good ventilation/exhaustion at the workplace.

Information about fire - and explosion protection:
Keep ignition sources away - Do not smoke.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles:
No special requirements.

Information about storage in one common storage facility:
Store away from oxidizing agents.
Do not store together with acids.

Further information about storage conditions:
Keep container tightly sealed.
Store in cool, dry conditions in well sealed receptacles.

Specific end use(s)

An important synthetic raw material, used as pharmaceutical intermediates.
Control parameters:

Ingredients with limit values that require monitoring at the workplace: Not required.

Additional information: The lists valid during the making were used as basis.

Exposure controls:

Personal protective equipment:

General protective and hygienic measures:
The usual precautionary measures are to be adhered to when handling chemicals.

Respiratory protection:
Use breathing protection with high concentration.

Protection of hands

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

Material of gloves
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Penetration time of glove material
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection:
Safety glasses
Face protection

Body protection:
Protective work clothing
09  Physical and Chemical Properties

Information on basic physical and chemical properties

General Information

Appearance:
- Form: Liquid
- Colour: Colourless

Odour:
- Odour: Characteristic
- Odour threshold: Not determined

pH-value:
- Not determined.

Change in condition
- Melting point/Melting range: -38°C
- Boiling point/Boiling range: 71-72°C (11 mm Hg)

Flash point:
- 76°C

Ignition temperature:
- 390°C

Decomposition temperature:
- Not determined.

Self-igniting:
- Not determined.

Danger of explosion:
- Product does not present an explosion hazard.

Explosion limits:
- Lower: Not determined.
- Upper: Not determined.

Vapour pressure:
- Not determined

Density at 20°C:
- 0.961 g/cm³

Relative density
- Not determined.

Vapour density
- Not determined.

Evaporation rate
- Not applicable.

Solubility in / Miscibility with water at 20°C:
- 9 g/l

Segregation coefficient (n-octanol/water):
- Not determined.

Viscosity:
- Dynamic: Not determined.
- Kinematic: Not determined.

Other information
- No further relevant information available.
10 Stability and reactivity

Reactivity

Chemical stability:

Thermal decomposition / conditions to be avoided:
No decomposition if used according to specifications.

Possibility of hazardous reactions
No dangerous reactions known.

Conditions to avoid
No further relevant information available

Incompatible materials:
Oxidizing agents
Acids

Hazardous decomposition products:
Oxides of carbon

11 Toxicological information

Information on toxicological effects
Acute Toxicity

LD/LC50 values relevant for classification:
Oral LD50 > 2000 mg/kg (rat)

Primary irritant effect:
on the skin: No irritant effect.
on the eye: No irritating effect.
Sensitization: No sensitizing effects known.

Additional toxicological information:
When used and handled according to specifications, the product does not have any harmful effects to our experience and the information provided to us.
The substance is not subject to classification according to the latest version of the EU lists.
12 Ecological Information

Toxicity

Acquatic toxicity:
No further relevant information available.

Persistence and degradability
No further relevant information available.

Behaviour in environmental systems:
Bioaccumulative potential
No further relevant information available.

Mobility in soil
No further relevant information available.

Additional ecological information:
General notes:
Water hazard class 1 (German Regulation) (Self-assessment): slightly hazardous for water
Do not allow product to reach ground water, water course or sewage system.

Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.

Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods

Recommendation:
Smaller quantities can be disposed of with household waste.

European waste catalogue
07 05 wastes from the MFSU of pharmaceuticals

Uncleaned packaging:
Recommendation: Disposal must be made according to official regulations.
14 Transport Information

Land transport ADR/RID (cross-border)
ADR/RID class: -

Maritime transport IMDG:
IMDG Class: -
Marine pollutant: No

Air transport ICAO-TI and IATA-DGR:
ICAO/IATA Class: -

UN "Model Regulation": -

Special precautions for user Not applicable.

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code
Not applicable

15 Regulatory Information

Labelling according to regulation (EC) No 1272/2008

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

Other regulations, limitations and prohibitive regulations

Substances of very high concern (SVHC) according to REACH, Article 57
The substance is not listed as SVHC.

Chemical safety assessment:
A Chemical Safety Assessment shall be carried out at the time of REACH Registration.
16 Other Information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

Abbreviations and acronyms

ADR : Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
RID : Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)
IMDG : International Maritime Code for Dangerous Goods
IATA : International Air Transport Association
IATA-DGR : Dangerous Goods Regulations by the "International Air Transport Association" (IATA)
ICAO : International Civil Aviation Organization
ICAO-TI : Technical Instructions by the "International Civil Aviation Organization" (ICAO)
GHS : Globally Harmonized System of Classification and Labelling of Chemicals
EINECS : European Inventory of Existing Commercial Chemical Substances
CAS : Chemical Abstracts Service (division of the American Chemical Society)
*Data compared to the previous version altered.*

Section 2 : Hazard Identification – Changes in classification and Labelling

Section 6 : Accidental Release Measures

Section 7 : Handling and Storage

Section 8 : Exposure Controls / Personal Protection

Section 9 : Physical and Chemical Properties

Section 10 : Stability and Reactivity

Section 11 : Toxicological Information

Section 12 : Ecological Information

Section 13 : Disposal Considerations