

# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** 4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone

### 1.2 Other means of identification

**Product number** -  
**Other names** KETONE MOSCHUS; 4-acetyl-1-tert-butyl-3,5-dimethyl-2-nitro-6-aminobenzene; 2-acetyl-5-tert-butyl-4,6-dinitroxylen

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.  
**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Baishun Biotechnology Co., Ltd  
**Address** No. 26, Lane 918, Lianye Road, Zhelin Town, Fengxian District, Shanghai, 201400, China  
**Telephone** +86-21-37581181

### 1.5 Emergency phone number

**Emergency phone number** +86-21-37581181  
**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Carcinogenicity, Category 2  
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

### 2.2 GHS label elements, including precautionary statements

**Pictogram(s)**



**Signal word** Warning  
**Hazard statement(s)** H351 Suspected of causing cancer  
H410 Very toxic to aquatic life with long lasting effects  
**Precautionary statement(s)**

<b>Prevention</b>	P203 Obtain, read and follow all safety instructions before use. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P273 Avoid release to the environment.
<b>Response</b>	P318 IF exposed or concerned, get medical advice. P391 Collect spillage.
<b>Storage</b>	P405 Store locked up.
<b>Disposal</b>	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

### 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	81-14-1	201-328-9	100%

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## SECTION 4: First-aid measures

### 4.1 Description of necessary first-aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### 4.2 Most important symptoms/effects, acute and delayed

no data available

### 4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

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## SECTION 5: Fire-fighting measures

### 5.1 Suitable extinguishing media

Fires involving this compound should be controlled using a Halon, carbon dioxide or dry chemical extinguisher. (NTP, 1992)

## 5.2 Specific hazards arising from the chemical

Flash point data is not available for this compound, however, it is probably combustible. (NTP, 1992)

## 5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### 6.2 Environmental precautions

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

### 6.3 Methods and materials for containment and cleaning up

SRP: Wastewater from contaminant suppression, cleaning of protective clothing/equipment, or contaminated sites should be contained and evaluated for subject chemical or decomposition product concentrations. Concentrations shall be lower than applicable environmental discharge or disposal criteria. Alternatively, pretreatment and/or discharge to a POTW is acceptable only after review by the governing authority. Due consideration shall be given to remediation worker exposure (inhalation, dermal and ingestion) as well as fate during treatment, transfer and disposal. If it is not practicable to manage the chemical in this fashion, it must meet Hazardous Material Criteria for disposal.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### 8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### 8.3 Individual protection measures, such as personal protective equipment (PPE)

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties and safety characteristics

Physical state	PHYSICAL DESCRIPTION: Light yellow crystalline solid. Insoluble in water. (NTP, 1992)
Colour	Yellow crystals
Odour	Unique ... powdery
Melting point/freezing point	135-139°C
Boiling point or initial boiling point and boiling range	369°C at 760 mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	153.2°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Insoluble (<1 mg/ml at 68.0° F) (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 4.30
Vapour pressure	5.84X10 <sup>-7</sup> mm Hg at 25 deg C (est)
Density and/or relative density	1.206 g/cm <sup>3</sup>
Relative vapour density	no data available
Particle characteristics	no data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

A nitrated ketone. Ketones are reactive with many acids and bases liberating heat and flammable gases (e.g., H<sub>2</sub>). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H<sub>2</sub>) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO<sub>3</sub>, HNO<sub>3</sub> + H<sub>2</sub>O<sub>2</sub>, and HClO<sub>4</sub>.

### 10.4 Conditions to avoid

no data available

## **10.5 Incompatible materials**

no data available

## **10.6 Hazardous decomposition products**

When heated to decomposition it emits toxic vapors of NO<sub>x</sub>.

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# **SECTION 11: Toxicological information**

### **Acute toxicity**

- Oral: LD50 Rat oral >10 g/kg
- Inhalation: no data available
- Dermal: no data available

### **Skin corrosion/irritation**

no data available

### **Serious eye damage/irritation**

no data available

### **Respiratory or skin sensitization**

no data available

### **Germ cell mutagenicity**

no data available

### **Carcinogenicity**

no data available

### **Reproductive toxicity**

no data available

### **STOT-single exposure**

no data available

### **STOT-repeated exposure**

no data available

### **Aspiration hazard**

no data available

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# **SECTION 12: Ecological information**

## **12.1 Toxicity**

- Toxicity to fish: no data available
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

## **12.2 Persistence and degradability**

AEROBIC: Musk ketone, present at 39 mg/L, reached 0% of its theoretical BOD in 28 days using an activated sludge inoculum at 100 mg/L in the Japanese MITI II test(1).

## **12.3 Bioaccumulative potential**

A BCF of 1,380 was measured in fish for musk ketone using rainbow trout (*Onchorynchus mykiss*) which were exposed over an 821-day period(1). According to a classification

scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is very high(SRC).

## 12.4 Mobility in soil

The Koc of musk ketone is estimated as 8,700(SRC), using a log Kow of 4.3(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that musk ketone is expected to be immobile in soil.

## 12.5 Other adverse effects

no data available

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# SECTION 13: Disposal considerations

## 13.1 Disposal methods

### Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

### Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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# SECTION 14: Transport information

## 14.1 UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## 14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## 14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## 14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## 14.5 Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

## 14.6 Special precautions for user

no data available

## 14.7 Transport in bulk according to IMO instruments

no data available

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# SECTION 15: Regulatory information

## 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	81-14-1	201-328-9
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

## SECTION 16: Other information

### Information on revision

**Creation Date** July 15, 2019

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### Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

### References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisys.com](mailto:sds@xixisys.com)**

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