



Safety Data Sheet  
Musk ketone

### 1. Identification

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Product name:	Musk ketone
Catalog#:	MSI6206AF
IUPAC name:	1-(4-tert-butyl-2,6-dimethyl-3,5-dinitrophenyl)ethanone
Product use restrictions:	Only for research and development use by, or directly under the supervision of, a technically qualified individual.
Company:	MetaSci Inc. 1 Yonge St., Suite 1801 Toronto, M5E 1W7, ON, Canada
Telephone:	(510) 429-8835
Website:	www.metasci.ca
Emergency contact number:	1-800-633-8253 United States & Canada 1-801-629-0667 International

### 2. Hazard Identification

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GHS Classification

Carcinogenicity (Category 2)

Short-term (acute) aquatic hazard (Category 1)

Long-term (chronic) aquatic hazard (Category 1)

Pictogram



Signal word  
Warning

Hazard statement(s)

H351

Suspected of causing cancer.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P273

Avoid release to the environment.

P281

Use personal protective equipment as required.

P308+P313

IF EXPOSED or concerned: Get medical advice/attention.

P391

Collect spillage.

P405

Store locked up.



P501

Dispose of contents/container to an approved waste disposal plant.

Hazards not otherwise classified (HNOC) or not covered by GHS  
None

### 3. Composition/Information on Ingredients

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Synonyms: 1-Acetyl-4-(tert-butyl)-2,6-dimethyl-3,5-dinitrobenzene  
CAS#: 81-14-1  
Purity: 99% (HPLC, GC)  
EC#: 201-328-9

### 4. First Aid Measures

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General information: Immediately remove any clothing contaminated by the product. Move out of dangerous area. Consult a physician and show this safety data sheet.

Inhalation: Move person to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Obtain medical aid.

Skin contact: Immediately flush skin with running water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Obtain medical aid immediately.

Eye contact: Immediately flush open eyes with running water for at least 15 minutes. Obtain medical aid immediately.

Ingestion: Do NOT induce vomiting without medical advice. Rinse mouth with water. Never administer anything by mouth to an unconscious person. Obtain medical aid immediately.

Most important symptoms and effects, both acute and delayed: No further information available. Please see sections 2 and 11.

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

### 5. Fire Fighting Measures

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Suitable extinguishing media: Use water spray, dry chemical, carbon dioxide, or chemical foam.

Specific hazards arising from the chemical: Nitrogen oxides, Carbon oxides

Advice for firefighters: As in any fire, wear a NIOSH-approved or equivalent, pressure-demand, self-contained breathing apparatus and full protective gear. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion.

### 6. Accidental Release Measures

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Personal precautions, protective equipment and emergency procedures: Wear protective equipment and keep unprotected personnel away. Ensure adequate ventilation. Remove all sources of ignition. Prevent further leak or spill if safe to do so. For personal protective equipment, please refer to section 8.

Environmental precautions: Do not let product enter drains, other waterways, or soil.



Methods and materials for containment and cleaning up: Prevent further leak or spill if safe to do so. Vacuum, sweep up, or absorb with inert material and place into a suitable disposal container. Consult local regulations for disposal. See section 13 for further disposal information.

## 7. Handling and Storage

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Precautions for safe handling: Avoid contact with skin, eyes, and personal clothing. Wash hands thoroughly after handling. Avoid breathing fumes. Use only with adequate ventilation. Wear suitable protective clothing, gloves, and eye/face protection. Keep away from sources of ignition. Minimize dust generation and accumulation. Keep container tightly closed. Open and handle container with care. Do not eat, drink, or smoke while handling.

Conditions for safe storage, including any incompatibilities: Store in a tightly-closed container when not in use. Store in a cool, dry, well-ventilated area away from incompatible substances. Keep away from sources of ignition. Error, no match for Store long-term in a cool, dry place

## 8. Exposure Controls/Personal Protection

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### Exposure limits

OSHA PEL: No data available.  
NIOSH REL: No data available.  
ACGIH TLV: No data available.

Appropriate engineering controls: Avoid contact with skin, eyes, and clothing. Wash hands before breaks and immediately after handling the product. Facilities storing or utilizing this material should be equipped with an eyewash fountain. Use adequate general and local exhaust ventilation to keep airborne concentrations low.

### 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 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: Respirators are not a substitute for accepted engineering control measures such as enclosure or confinement of the operation, general and local ventilation, and substitution of less toxic



materials. When respiratory personal protective equipment is appropriate based on an assessment of respiratory hazards in the workplace, use a NIOSH- or CEN-certified respirator.

## 9. Physical and Chemical Properties

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Physical State:	Solid
Molecular Formula:	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>
Molecular Weight:	294.31
Odor:	No data available.
pH:	No data available.
Boiling Point Range:	No data available.
Freezing/Melting Point:	135-139 °C (lit.)
Flash Point:	> 168 °C (> 334 °F) - closed cup
Evaporation Rate:	No data available.
Flammability (solid, gas):	Please see section 2.
Explosive limits:	No data available.
Vapor Pressure:	0.1 hPa at 80 °C (176 °F)
Vapor Density:	No data available.
Solubility:	water:0.00046 g/l at 20 °C (68 °F);
Relative Density:	No data available.
Refractive Index:	No data available.
Volatility:	No data available.
Auto-ignition temperature:	No data available.
Decomposition Temperature:	No data available.
Partition Coefficient:	No data available.

## 10. Stability and Reactivity

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Reactivity:	No data available.
Chemical stability:	Stable under recommended temperatures and pressures.
Possibility of hazardous reactions:	No data available.
Conditions to avoid:	Dust generation. Heat.
Incompatible materials:	Strong oxidizing agents.
Hazardous decomposition products:	Nitrogen oxides, Carbon oxides

## 11. Toxicological Information

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RTECS#:	KM5775841
Acute toxicity:	LD <sub>50</sub> Oral: Rat - > 10,000 mg/kg; LD <sub>50</sub> Dermal: Rabbit - > 10,000 mg/kg;
Routes of exposure:	Inhalation, eye contact, skin contact, ingestion.



Symptoms related to the physical, chemical and toxicological characteristics: Skin contact may result in inflammation characterized by itching, scaling, reddening, blistering, pain or dryness. Eye contact may result in redness, pain or severe eye damage. Inhalation may cause irritation of the lungs and respiratory system. Overexposure may result in serious illness or death.

Carcinogenicity

IARC: Not classified.

NTP: Not listed.

OSHA: Not listed.

Acute toxic effects: Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

## 12. Ecological Information

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Ecotoxicity: Toxicity to algae: Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 0.24 mg/l - 72 h (OECD Test Guideline 201) NOEC - Pseudokirchneriella subcapitata (green algae) - 0.088 mg/l - 72 h (OECD Test Guideline 201)  
Toxicity to daphnia and other aquatic invertebrates: static test - Daphnia magna (Water flea) - > 0.46 mg/l - 48 h (OECD Test Guideline 202)

Persistence and degradability: No data available.

Bioaccumulative potential: No data available.

Mobility in soil: No data available.

Other adverse effects: No data available.

## 13. Disposal Considerations

Disposal of waste: Chemical waste generators must determine whether a discarded chemical is classified as hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification. Observe all federal, state and local regulations when disposing of the substance.

Disposal of packaging: Do not reuse containers. Dispose of as unused product.

## 14. Transportation Information

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DOT (United States)

UN number: Not hazmat

Proper shipping name: Not applicable.

Transport hazard class: Not applicable.

Packing group: Not applicable.



#### IATA

UN number: UN3077  
Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (Musk ketone)  
Transport hazard class: 9  
Packing group: III

#### 15. Regulatory Information

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##### TSCA Chemical Inventory:

This product is on the EPA Toxic Substance Control Act (TSCA) inventory. The product is supplied solely for use in research and development by or under the supervision of a technically qualified individual as defined in 40 CFR § 720 et seq. The health risks have not been fully determined. Any information that is or becomes available will be supplied on the SDS.

Canada  
DSL/NDSL: This product is listed in the Domestic Substance List (DSL).

California

Proposition 65:

NFPA Rating:	Health:	No data available.
	Flammability:	No data available.
	Instability:	No data available.

#### 16. Additional Information

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##### Disclaimer:

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