

SAFETY DATA SHEET

Version 3.14
Revision Date 06/25/2014
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Musk ketone

Product Number : W522902

Brand : Aldrich

CAS-No. : 81-14-1

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Carcinogenicity (Category 2), H351

Acute aquatic toxicity (Category 1), H400

Chronic aquatic toxicity (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

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.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Ketone Moschus
4-tert-Butyl-2,6-dimethyl-3,5-dinitroacetophenone

Formula : C₁₄H₁₈N₂O₅

Molecular Weight : 294.3 g/mol

CAS-No. : 81-14-1

Hazardous components

Component	Classification	Concentration
4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone		
	Carc. 2; Aquatic Acute 1; Aquatic Chronic 1; H351, H410	90 - 100 %
Musk xylene Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)		
	Expl. 1.2; Carc. 2; Aquatic Acute 1; Aquatic Chronic 1; H202, H351, H410	0.1 - 1 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO_x)

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions

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

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: crystalline Colour: yellow
b) Odour	no data available
c) Odour Threshold	no data available
d) pH	no data available
e) Melting point/freezing point	Melting point/range: 135 - 139 °C (275 - 282 °F) - lit.
f) Initial boiling point and boiling range	no data available
g) Flash point	> 168 °C (> 334 °F) - closed cup
h) Evaporation rate	no data available
i) Flammability (solid, gas)	no data available
j) Upper/lower flammability or explosive limits	no data available
k) Vapour pressure	0.1 hPa (0.1 mmHg) at 80 °C (176 °F)
l) Vapour density	no data available
m) Relative density	no data available
n) Water solubility	0.00046 g/l at 20 °C (68 °F)
o) Partition coefficient: n-octanol/water	log Pow: 4.3
p) Auto-ignition temperature	no data available
q) Decomposition temperature	no data available
r) Viscosity	no data available
s) Explosive properties	no data available
t) Oxidizing properties	no data available

9.2 Other safety information

no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

no data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong acids, Strong bases

10.6 Hazardous decomposition products

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - rat - > 10,000 mg/kg

Inhalation: no data available

LD50 Dermal - rabbit - > 10,000 mg/kg

no data available

Skin corrosion/irritation

Skin - rabbit

Result: No skin irritation - 24 h

Serious eye damage/eye irritation

Eyes - guinea pig

Result: No eye irritation - 24 h

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Suspected human carcinogens

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Musk xylene)

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

no data available

Reproductive toxicity - rat - Oral

Maternal Effects: Other effects. Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

Reproductive toxicity - rat - Oral

Maternal Effects: Other effects. Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

no data available

Specific target organ toxicity - single exposure

no data available

Specific target organ toxicity - repeated exposure

no data available

Aspiration hazard

no data available

Additional Information

RTECS: KM5775841

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates	static test - Daphnia magna (Water flea) - > 0.46 mg/l - 48 h (OECD Test Guideline 202)
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)

12.2 Persistence and degradability

Biodegradability	aerobic Biochemical oxygen demand - Exposure time 28 d Result: < 80 % - Not readily biodegradable. (OECD Test Guideline 302)
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12.3 Bioaccumulative potential

Bioaccumulation	Oncorhynchus mykiss (rainbow trout) - 21 d - 47 µg/l Bioconcentration factor (BCF): 1,380
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12.4 Mobility in soil

no data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

UN number: 3077 Class: 9 Packing group: III EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone)
Marine pollutant: Marine pollutant

IATA

UN number: 3077 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone)

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

15. REGULATORY INFORMATION

SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	81-14-1	

New Jersey Right To Know Components

	CAS-No.	Revision Date
4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone	81-14-1	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Carc.	Carcinogenicity
Expl.	Explosives
H202	Explosive, severe projection hazard.
H351	Suspected of causing cancer.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

HMIS Rating

Health hazard:	0
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	0
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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