1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

<table>
<thead>
<tr>
<th>Product name</th>
<th>Musk ketone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Number</td>
<td>W522902</td>
</tr>
<tr>
<td>Brand</td>
<td>Aldrich</td>
</tr>
<tr>
<td>REACH No.</td>
<td></td>
</tr>
<tr>
<td>A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.</td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>81-14-1</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Company</th>
<th>Sigma-Aldrich</th>
</tr>
</thead>
<tbody>
<tr>
<td>3050 Spruce Street</td>
<td></td>
</tr>
<tr>
<td>SAINT LOUIS MO  63103</td>
<td></td>
</tr>
<tr>
<td>USA</td>
<td></td>
</tr>
<tr>
<td>Telephone</td>
<td>+1 800-325-5832</td>
</tr>
<tr>
<td>Fax</td>
<td>+1 800-325-5052</td>
</tr>
</tbody>
</table>

1.4 Emergency telephone number

| Emergency Phone # | (314) 776-6555 |

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

<table>
<thead>
<tr>
<th>Signal word</th>
<th>Warning</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hazard statement(s)</td>
<td></td>
</tr>
<tr>
<td>H351</td>
<td>Suspected of causing cancer.</td>
</tr>
<tr>
<td>H410</td>
<td>Very toxic to aquatic life with long lasting effects.</td>
</tr>
<tr>
<td>Precautionary statement(s)</td>
<td></td>
</tr>
<tr>
<td>P201</td>
<td>Obtain special instructions before use.</td>
</tr>
<tr>
<td>P202</td>
<td>Do not handle until all safety precautions have been read and understood.</td>
</tr>
<tr>
<td>P273</td>
<td>Avoid release to the environment.</td>
</tr>
<tr>
<td>P281</td>
<td>Use personal protective equipment as required.</td>
</tr>
<tr>
<td>P308 + P313</td>
<td>IF exposed or concerned: Get medical advice/attention.</td>
</tr>
</tbody>
</table>
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:
C_{14}H_{18}N_{2}O_{5}

Molecular Weight:
294.30 g/mol

CAS-No.:
81-14-1

Hazardous components

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone</td>
<td>Carc. 2; Aquatic Acute 1; Aquatic Chronic 1; H351, H410</td>
<td>90 - 100 %</td>
</tr>
</tbody>
</table>

Musk xylene Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Musk xylene</td>
<td>Expl. 1.2; Carc. 2; Aquatic Acute 1; Aquatic Chronic 1; H202, H351, H410</td>
<td>0.1 - 1 %</td>
</tr>
</tbody>
</table>

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 (NOx)

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.
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
In the event of fire: see section 5

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)

12.3 Bioaccumulative potential

Bioaccumulation Oncorhynchus mykiss (rainbow trout) - 21 d - 47 µg/l

Bioconcentration factor (BCF): 1,380

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

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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
Chroni Health Hazard

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

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>4'-tert-Butyl-2',6'-dimethyl-3',5'-dinitroacetophenone</td>
<td>81-14-1</td>
<td></td>
</tr>
</tbody>
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New Jersey Right To Know Components

<table>
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<tr>
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<th>CAS-No.</th>
<th>Revision Date</th>
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<tbody>
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<td>81-14-1</td>
<td></td>
</tr>
</tbody>
</table>

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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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the
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Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 3.10  Revision Date: 01/17/2014  Print Date: 01/29/2014