

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Nootkatone  
  
Product Number : W316620  
Brand : Aldrich  
  
CAS-No. : 4674-50-4

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

Identified uses : Laboratory chemicals, Synthesis 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)

Skin sensitisation (Category 1), H317

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)

H317

May cause an allergic skin reaction.

Precautionary statement(s)

P261

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

P272

Contaminated work clothing should not be allowed out of the workplace.

P280

Wear protective gloves.

P302 + P352

IF ON SKIN: Wash with plenty of soap and water.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P363

Wash contaminated clothing before reuse.

P501

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

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

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Formula : C<sub>15</sub>H<sub>22</sub>O  
Molecular weight : 218.33 g/mol  
CAS-No. : 4674-50-4  
EC-No. : 225-124-4

#### Hazardous components

| Component             | Classification     | Concentration |
|-----------------------|--------------------|---------------|
| <b>(+)-Nootkatone</b> | Skin Sens. 1; H317 | 90 - 100 %    |

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

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### 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

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### 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

No data available

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

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### 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. Avoid breathing dust.

For personal protection see section 8.

#### 6.2 Environmental precautions

Do not let product enter drains.

### 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.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. 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.

Recommended storage temperature 2 - 8 °C

Storage class (TRGS 510): 13: Non Combustible Solids

### 7.3 Specific end use(s)

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

Hazardous components without workplace control parameters

### 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

Face shield and safety glasses 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

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |               |  |
|---------------|--|
| a) Appearance | Form: crystalline<br>Colour: white, light yellow |
| b) Odour      | citrus, slight, woody                            |

|   |  |
|---|--|
| c) Odour Threshold                              | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | Melting point/freezing point: $\geq 32$ °C ( $\geq 90$ °F) |
| f) Initial boiling point and boiling range      | No data available  |
| g) Flash point                                  | ca.140 °C (284 °F)   |
| 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                              | ca.< 0.001 hPa (< 0.001 mmHg) at 25 °C (77 °F)             |
| l) Vapour density                               | No data available  |
| m) Relative density                             | 0.97 - 1.032 g/cm <sup>3</sup> at 25 °C (77 °F)            |
| n) Water solubility                             | practically insoluble                                      |
| o) Partition coefficient: n-octanol/water       | log Pow: ca.4 at 25 °C (77 °F)                             |
| 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

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## 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 oxidizing agents, Strong acids and strong bases

### 10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - > 5,000 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - > 5,000 mg/kg

No data available

**Skin corrosion/irritation**

No data available

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitisation**

No data available

**Germ cell mutagenicity**

No data available

Ames test

Result: negative

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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 on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

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: Not available

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

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**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

Biodegradability Result: 65 % - Not readily biodegradable.

**12.3 Bioaccumulative potential**

No data available

**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**

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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## 15. REGULATORY INFORMATION

**SARA 302 Components**

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

**SARA 313 Components**

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**

Acute 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 |
|----------------|-----------|---------------|
| (+)-Nootkatone | 4674-50-4 |               |

**New Jersey Right To Know Components**

|                | CAS-No.   | Revision Date |
|----------------|-----------|---------------|
| (+)-Nootkatone | 4674-50-4 |               |

**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.

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## 16. OTHER INFORMATION

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

|            |                                      |
|------------|--------------------------------------|
| H317       | May cause an allergic skin reaction. |
| Skin Sens. | Skin sensitisation                   |

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: |   |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 0 |
| 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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