

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 1 of 7

#### SECTION 1: Identification of the substance/mixture and of the company/undertaking

##### 1.1. Product identifier

4-(3,6-Dimethyl-3-heptyl)phenol-13C6

CAS No: 1173020-38-6

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

###### Use of the substance/mixture

Reference standard for analysis.

##### 1.3. Details of the supplier of the safety data sheet

Company name: WITEGA Laboratorien Berlin-Adlershof GmbH  
Street: James-Franck-Strasse 4  
Place: D-12489 Berlin  
Telephone: +493063922001      Telefax: +493063922007  
e-mail: witega@witega.de  
Internet: www.witega.de

**1.4. Emergency telephone number:** +493063922001

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

###### GB CLP Regulation

Repr. 2; H361  
Acute Tox. 4; H302  
Skin Irrit. 2; H315  
Eye Irrit. 2B; H320  
STOT SE 3; H335  
Aquatic Acute 1; H400  
Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

##### 2.2. Label elements

###### GB CLP Regulation

**Signal word:** Warning

**Pictograms:**



###### Hazard statements

|           |   |
|-----------|---|
| H302      | Harmful if swallowed.                                 |
| H335      | May cause respiratory irritation.                     |
| H315+H320 | Causes skin and eye irritation.                       |
| H361      | Suspected of damaging fertility or the unborn child.  |
| H400      | Very toxic to aquatic life.                           |
| H410      | Very toxic to aquatic life with long lasting effects. |

###### Precautionary statements

|                |  |
|----------------|--|
| P281           | Use personal protective equipment as required.   |
| P262           | Do not get in eyes, on skin, or on clothing.   |
| P261           | Avoid breathing dust/fume/gas/mist/vapours/spray.                                      |
| P305+P351+P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if |

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 2 of 7

present and easy to do. Continue rinsing.

#### 2.3. Other hazards

No data available

### SECTION 3: Composition/information on ingredients

#### 3.1. Substances

Sum formula: C<sub>9</sub>H<sub>24</sub>O 13C<sub>6</sub>

Molecular weight: 226.31 g/mol

#### Hazardous components

| CAS No       | Chemical name   | Quantity |          |  |
|--------------|---|----------|----------|--|
|              | EC No   | Index No | REACH No |  |
|              | Classification (GB CLP Regulation)  |          |          |  |
| 1173020-38-6 | 4-(3,6-Dimethyl-3-heptyl)phenol-13C6  | 100 %    |          |  |
|              | Repr. 2, Acute Tox. 4, Skin Irrit. 2, Eye Irrit. 2B, STOT SE 3, Aquatic Acute 1, Aquatic Chronic 1;<br>H361 H302 H315 H320 H335 H400 H410 |          |          |  |

Full text of H and EUH statements: see section 16.

#### Specific Conc. Limits, M-factors and ATE

| CAS No       | EC No                                    | Chemical name                        | Quantity |
|--------------|--|--------------------------------------|----------|
|              | Specific Conc. Limits, M-factors and ATE |                                      |          |
| 1173020-38-6 |  | 4-(3,6-Dimethyl-3-heptyl)phenol-13C6 | 100 %    |
|              | oral: ATE = 500 mg/kg                    |                                      |          |

### SECTION 4: First aid measures

#### 4.1. Description of first aid measures

##### General information

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

##### After inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

##### After contact with skin

Remove contaminated, saturated clothing immediately. Subsequently wash off with: Water and soap

##### After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

##### After ingestion

Rinse mouth immediately and drink plenty of water. Get immediate medical advice/attention.

Do NOT induce vomiting. Never give anything by mouth to an unconscious person or a person with cramps.

#### 4.2. Most important symptoms and effects, both acute and delayed

No data available

#### 4.3. Indication of any immediate medical attention and special treatment needed

No data available

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

##### Suitable extinguishing media

Water spray jet. Foam. Dry extinguishing powder. Carbon dioxide (CO<sub>2</sub>).

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 3 of 7

#### **5.2. Special hazards arising from the substance or mixture**

In case of fire may be liberated: Pyrolysis products, toxic. In case of fire and/or explosion do not breathe fumes.

#### **5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

### **SECTION 6: Accidental release measures**

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

##### **General advice**

Use personal protection equipment. Do not breathe gas/fumes/vapour/spray.

#### **6.2. Environmental precautions**

Do not allow to enter into surface water or drains.

#### **6.3. Methods and material for containment and cleaning up**

##### **Other information**

Take up dust-free and set down dust-free.

#### **6.4. Reference to other sections**

Disposal: see section 13

### **SECTION 7: Handling and storage**

#### **7.1. Precautions for safe handling**

##### **Advice on safe handling**

If handled uncovered, arrangements with local exhaust ventilation should be used if possible.

##### **Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

##### **Advice on general occupational hygiene**

Use personal protection equipment.

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

##### **Requirements for storage rooms and vessels**

Keep container tightly closed in a cool, well-ventilated place. Avoid: UV-radiation/sunlight

##### **Further information on storage conditions**

storage temperature: 2-8°C

#### **7.3. Specific end use(s)**

none

### **SECTION 8: Exposure controls/personal protection**

#### **8.1. Control parameters**

#### **8.2. Exposure controls**

##### **Appropriate engineering controls**

If handled uncovered, arrangements with local exhaust ventilation should be used if possible. If local exhaust ventilation is not possible or not sufficient, the entire working area should be ventilated by technical means.

##### **Individual protection measures, such as personal protective equipment**

##### **Eye/face protection**

Eye glasses with side protection

##### **Hand protection**

Wear suitable gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances.

##### **Skin protection**

lab coat

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 4 of 7

#### Respiratory protection

In case of inadequate ventilation wear respiratory protection.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

|   |            |                   |
|---|------------|-------------------|
| Physical state:   | Liquid     |                   |
| Colour:   | colourless |                   |
| Odour:  | odourless  |                   |
| Melting point/freezing point:                             |            | No data available |
| Boiling point or initial boiling point and boiling range: |            | No data available |
| Flammability:   |            | No data available |
| Lower explosion limits:                                   |            | No data available |
| Upper explosion limits:                                   |            | No data available |
| Flash point:  |            | No data available |
| Auto-ignition temperature:                                |            | No data available |
| Decomposition temperature:                                |            | No data available |
| pH-Value:   |            | No data available |
| Water solubility:   |            | No data available |
| Solubility in other solvents                              |            |                   |
| No data available   |            |                   |
| Partition coefficient n-octanol/water:                    |            | No data available |
| Vapour pressure:  |            | No data available |
| Density:  |            | No data available |
| Relative vapour density:                                  |            | No data available |

#### 9.2. Other information

##### Information with regard to physical hazard classes

|                           |                   |
|---------------------------|-------------------|
| Explosive properties      |                   |
| No data available         |                   |
| Self-ignition temperature |                   |
| Solid:                    | No data available |
| Gas:                      | No data available |
| Oxidizing properties      |                   |
| No data available         |                   |

##### Other safety characteristics

|                   |                   |
|-------------------|-------------------|
| Evaporation rate: | No data available |
|-------------------|-------------------|

##### Further Information

none

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

Reacts with : Oxidising agent, Alkali (lye), Etchant and acids

#### 10.2. Chemical stability

The product is chemically stable under recommended conditions of storage, use and temperature.

#### 10.3. Possibility of hazardous reactions

No known hazardous reactions.

#### 10.4. Conditions to avoid

Do not expose to temperatures exceeding 50 °C/122 °F.

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 5 of 7

#### 10.5. Incompatible materials

Oxidising agent, Alkali (lye), Etchant and acids

#### 10.6. Hazardous decomposition products

In case of fire may be liberated: Pyrolysis products, toxic.

### SECTION 11: Toxicological information

#### 11.1. Information on hazard classes as defined in GB CLP Regulation

##### Acute toxicity

Harmful if swallowed.

| CAS No       | Chemical name                        |               |         |        |        |
|--------------|--------------------------------------|---------------|---------|--------|--------|
|              | Exposure route                       | Dose          | Species | Source | Method |
| 1173020-38-6 | 4-(3,6-Dimethyl-3-heptyl)phenol-13C6 |               |         |        |        |
|              | oral                                 | ATE 500 mg/kg |         |        |        |

##### Irritation and corrosivity

Causes skin and eye irritation.

##### Sensitising effects

Based on available data, the classification criteria are not met.

##### Carcinogenic/mutagenic/toxic effects for reproduction

Suspected of damaging fertility or the unborn child. (4-(3,6-Dimethyl-3-heptyl)phenol-13C6)

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

##### STOT-single exposure

May cause respiratory irritation. (4-(3,6-Dimethyl-3-heptyl)phenol-13C6)

##### STOT-repeated exposure

Based on available data, the classification criteria are not met.

##### Aspiration hazard

Based on available data, the classification criteria are not met.

##### Specific effects in experiment on an animal

No data available

### SECTION 12: Ecological information

#### 12.1. Toxicity

No data available

#### 12.2. Persistence and degradability

No data available

#### 12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

#### 12.4. Mobility in soil

No data available

#### 12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of UK REACH.

This substance does not meet the PBT/vPvB criteria of REACH, Annex XIII.

#### 12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

#### 12.7. Other adverse effects

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 6 of 7

No data available

#### SECTION 13: Disposal considerations

##### 13.1. Waste treatment methods

###### Disposal recommendations

Dispose of waste according to applicable legislation.

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

###### Contaminated packaging

This material and its container must be disposed of as hazardous waste.

#### SECTION 14: Transport information

##### Land transport (ADR/RID)

**14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.

##### Inland waterways transport (ADN)

**14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.

##### Marine transport (IMDG)

**14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.

##### Air transport (ICAO-TI/IATA-DGR)

**14.2. UN proper shipping name:** No dangerous good in sense of this transport regulation.

##### 14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

##### 14.6. Special precautions for user

No data available

##### 14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

#### SECTION 15: Regulatory information

##### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

###### National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 3 - highly hazardous to water

##### 15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

#### SECTION 16: Other information

##### Relevant H and EUH statements (number and full text)

|           |   |
|-----------|---|
| H302      | Harmful if swallowed.                                 |
| H315      | Causes skin irritation.                               |
| H315+H320 | Causes skin and eye irritation.                       |
| H320      | Causes eye irritation.                                |
| H335      | May cause respiratory irritation.                     |
| H361      | Suspected of damaging fertility or the unborn child.  |
| H400      | Very toxic to aquatic life.                           |
| H410      | Very toxic to aquatic life with long lasting effects. |

## Safety Data Sheet

according to UK REACH Regulation

### 4-(3,6-Dimethyl-3-heptyl)phenol-13C6

Revision date: 16.02.2024

Product code: OP128

Page 7 of 7

#### Further Information

This information is based on our present state of knowledge. However, it should not constitute a guarantee for any specific product properties and shall not establish a legally valid relationship. The substances are only for R&D. Do not use as a drug, in household or other applications.