

# Firmenich

## GHS Safety Data Sheet

According to Regulation ST/SG/AC.10/30/Rev.8 UN GHS

This Safety Data Sheet cancels and replaces all preceding SDS for this product.

### **1 IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND OF THE COMPANY/UNDERTAKING**

#### 1.1 Product identifier

**966466**

NEOBUTENONE® ALPHA

© Firmenich product

CAS No: 56973-85-4  
EC No: 260-486-7  
EU REACH No: 01-2120735847-42

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

Fragrance ingredient for use in consumer products.  
Not for personal use in this form or concentration.  
Intended to be used in the manufacture of products for consumers

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

Firmenich Asia Private Ltd  
No 10 Tuas West Road  
Singapore 638377  
SINGAPORE  
Tel: +(65) 6347 2888

GRS.Fragrance.FIRSIN@firmenich.com

#### 1.4 Emergency telephone number

+65 3158 1074 NCEC - Available 24/7

### **2 HAZARDS IDENTIFICATION**

#### 2.1 Classification of the substance or mixture

##### 2.1.1 Classification according to Regulation ST/SG/AC.10/30/Rev.8 [UN/GHS]

|   |      |
|---|------|
| Acute Toxicity (oral) - Cat. 5          | H303 |
| Skin Sensitization - Cat. 1B            | H317 |
| Environmental Hazard (acute) - Cat. 2   | H401 |
| Environmental Hazard (chronic) - Cat. 2 | H411 |

##### 2.1.2 Additional information

Full text of listed statements : See section 16

#### 2.2 Label elements

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### Hazard pictograms:



### Signal Word:

Warning

### Hazard Statements:

H317 May cause an allergic skin reaction.  
H303 May be harmful if swallowed.  
H411 Toxic to aquatic life with long lasting effects.

### Precautionary Statements:

P261 Avoid breathing mist/vapours.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P273 Avoid release to the environment.  
P302+P352 IF ON SKIN: Wash with plenty of soap and water.  
P333+P313 If skin irritation or rash occurs: Get medical advice/attention.  
P391 Collect spillage.

### 2.3 Other hazards

No data available at this time.

## 3 COMPOSITION/INFORMATION ON INGREDIENTS

Chemical substance.

### Contains :

>= 99.0 <= 100.0%  
4-Penten-1-One, 1-(5,5-Dimethyl-1-Cyclohexen-1-Yl)-  
N° CAS : 0056973-85-4  
N° EINECS: 260-486-7  
N° EU REACH: 01-2120735847-42

### GHS Classification:

Skin Sensitization - Cat. 1B [H317]  
Environmental Hazard (chronic) - Cat. 2 [H411]  
Environmental Hazard (acute) - Cat. 2 [H401]  
Acute Toxicity (oral) - Cat. 5 [H303]

## 4 FIRST-AID MEASURES

### 4.1 Description of first aid measures

General information:

As in all cases of potential poisoning, Obtain medical advice immediately.

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In case of eye contact:

Irrigate copiously with water for at least 10 minutes. Obtain medical advice if any irritation or evidence of tissue damage persists.

In case of inhalation:

Remove the individual to fresh air and keep at rest. Obtain medical advice immediately.

In case of skin contact:

Remove contaminated clothes. Wash skin with large volumes of water.

If irritation persists, or any sign of tissue damage is apparent, obtain medical advice immediately.

In case of ingestion:

Rinse mouth with water. Obtain medical advice immediately.

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

No specific data available.

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

No specific data available.

### **5 FIRE-FIGHTING MEASURES**

#### 5.1 Extinguishing media

In the event of fire, adequate extinguishers should be used. Avoid inhalation of smoke and fumes. In case of insufficient ventilation, wear suitable respiratory equipment.

#### 5.2 Special hazard arising from the substance or mixture

No specific hazard known.

#### 5.3 Advice for fire-fighters

No specific advice.

### **6 ACCIDENTAL RELEASE MEASURES**

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

For non-emergency personnel:

Adequate protective gloves should be worn when handling spillages. No smoking. Avoid naked flames or other potential sources of ignition (eg. electrical equipment).

Avoid skin contamination and inhalation of vapour.

Individual washing routines should be followed after any potential contact.

Ensure adequate ventilation in working areas following accidental releases.

For emergency personnel:

Apply the same recommendations as section 6.1

#### 6.2 Environmental precautions

Do not discharge directly into drains, air, into soil or into the aquatic environment.

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

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For containment:

Any absorbent used for cleaning up spillage should be disposed promptly, accordingly to local regulation. Gross spillages should be contained by any means, and disposal of this should be in accordance with Government Regulations.

For cleaning-up:

Spillages should be disposed of in accordance with Governmental Regulations.

### **7 HANDLING AND STORAGE**

#### 7.1 Precautions for safe handling

Avoid contact with skin and eyes.

Wear adequate protective gloves protection and eye/face protection.

No smoking. Avoid any sources of ignition.

Avoid exposing to high temperature during processing.

Do not ingest or apply to the skin as such. Good personal washing routines should be followed.

Maintain adequate local and general ventilation where product is handled.

#### 7.1.1 Protective measures

Keep strict control of dust accumulation to a minimum. Maintain adequate local and general ventilation where product is handled. Avoid any sources of ignition.

#### 7.1.2 Advice on general occupational hygiene

Good personal washing routines should be followed.

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

It is good general practice to store in closed, preferably full, containers away from heat sources, and protected from extremes of temperature. Do not re-use the empty container.

Respect general rules for compatibility storage.

#### 7.3 Specific end use(s)

Not available at this time.

### **8 EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### 8.1 Control parameters

Contains no substances with occupational exposure limit values

#### **Derived No Effect Level (DNEL)**

DNEL Worker (dermal), systemic effects - long-term, = 0.714 mg/kg bw/day

Hazard conclusion Worker (dermal), local effects - acute & long-term, Medium hazard (no threshold derived) (sensitisation)

DNEL Worker (inhalation), systemic effects - long-term, = 2.52 mg/m<sup>3</sup>

DNEL Consumer (oral), systemic effects - long-term, = 0.255 mg/kg bw/day

DNEL Consumer (inhalation), systemic effects - long-term, = 0.377 mg/m<sup>3</sup>

DNEL Consumer (dermal), systemic effects - long-term, = 0.255 mg/kg bw/day

Hazard conclusion Consumer (dermal), local effects - acute & long-term, Medium hazard (no threshold derived) (sensitisation)

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### Predicted No Effect Concentration (PNEC)

PNEC Aqua (freshwater) = 1.7 µg/l  
PNEC Aqua (marine water) = 0.17 µg/l  
PNEC Water (intermittent release) freshwater = 17 µg/l  
PNEC Water (intermittent release) marine water = 1.7 µg/l  
PNEC Sediment (freshwater) = 0.242 mg/kg sediment dw  
PNEC Sediment (marine water) = 0.024 mg/kg sediment dw  
PNEC STP = 4.6 mg/l  
PNEC Soil = 0.047 mg/kg soil dw  
PNEC Air No hazard identified.  
PNEC Oral (secondary poisoning) = 5.67 mg/kg food

### 8.2 Exposure controls

Avoid exposing to high temperature during processing.  
Maintain adequate local and general ventilation where product is handled.

#### 8.2.1 Appropriate engineering controls

Maintain adequate local and general ventilation where product is handled and dispensed.

#### 8.2.2 Environmental exposure controls

Not available at this time. Minimize release to the environment.

### 8.3 Personal protection

Respiratory protection: Where ventilation (LEV) is inadequate to prevent any inhalation of substances, use adequate respiratory apparatus.

Hand protection: Adequate Protective Gloves should be worn.

Eye protection: Adequate safety glasses should be used.

Skin protection: Wear protective clothing, overall if necessary to limit the odour contamination of personal clothing. Individual washing routines should be followed after any potential contact.

## 9 PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|                                    |   |
|------------------------------------|---|
| Appearance :                       | LIQUID  |
| Colour :                           | COLOURLESS TO PALE YELLOW   |
| Odour :                            | Characteristic strong odour according to the commercial description of the substance. |
| pH :                               | Not available   |
| Melting point/range (°C) :         | < -20 °C (OECD 102)   |
| Initial boiling point/range (°C) : | = 265.9 °C (OECD 103)   |
| Flash point (closed cup) :         | = 112°C   |
| Evaporation rate :                 | Not available   |
| Flammability (solid/gas) :         | Not applicable  |
| Explosive properties (St class) :  | N/A   |
| Vapour pressure (Pa) :             | 1.43988408  |
| Vapour density :                   | Not available   |

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|                                     |                                |
|-------------------------------------|--------------------------------|
| Relative density (d 20/20) :        | = 0.925 at 20°C (OECD 109)     |
| Water solubility (20°C) :           | = 56.2 mg/l at 20°C (OECD 105) |
| Partition coef. (n-octanol/water) : | Log Kow = 4.1 (OECD 117)       |
| Auto-ignition temperature (°C) :    | Not available                  |
| Decomposition temperature :         | Not available                  |
| Viscosity :                         | Not available                  |
| Explosive properties :              | Not available                  |
| Oxidizing properties :              | Not available                  |

### 9.2 Other safety information

None

## **10 STABILITY AND REACTIVITY**

### 10.1 Reactivity

No reaction known with water.

### 10.2 Chemical stability

Good stability at standard temperature.

### 10.3 Possibility of hazardous reactions

Not known.

### 10.4 Conditions to avoid

Avoid temperatures above or at least 5 °C below flash point for any flammable liquids.

Do not heat closed containers.

Avoid contact with oxidizing agents.

### 10.5 Incompatible materials

Not known.

### 10.6 Hazardous decomposition products

Contact with water or storage under recommended conditions for one year should not produce dangerous decomposition products.

## **11 TOXICOLOGICAL INFORMATION**

### **11.1 Information on toxicological effects**

#### (a) acute toxicity

Acute oral toxicity (Rat, OECD 401, Gavage): LD50 > 2500 mg/kg

Data on analogue - Acute oral toxicity (Rat, Gavage): LD50 > 2000 mg/kg

Acute dermal toxicity : LD50 > 2500 mg/kg

#### (b) skin corrosion/irritation

Data on analogue - Primary Skin irritation (Rabbit, OECD 404, Semi-occlusive): Non irritant

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(c) serious eye damage/irritation

Isolated Chicken Eye test method for identifying ocular corrosives and severe irritant (OECD 438):

Non irritant

Data on analogue - Acute Eye irritation (Rabbit, OECD 405, No washout): Non irritant

(d) respiratory or skin sensitisation

Data on analogue - Guinea pig Maximisation test (OECD 406): Sensitising to skin

(e) germ cell mutagenicity

Bacterial Reverse Mutation test (Ames) (Salmonella + E. Coli, OECD 471, With and without S9, 5 strains): Non mutagenic

Data on analogue - In vitro Mammalian Cell Gene Mutation Tests Using the Thymidine Kinase Gene (OECD 490, Mouse lymphoma assay): Non mutagenic

Data on analogue - In vitro Mammalian Chromosome Aberration Test (Human, OECD 473): No chromosomal aberration

(f) carcinogenicity

No data available

(g) reproductive toxicity

Data on analogue - Combined Repeat. Dose Tox. & Reprod./Develop. Tox. Screening (Rat, OECD 422, Dietary, 91 day(s)):

NOAEL = 42 mg/kg/day

NOAEL (fertility) = 137 mg/kg/day

NOAEL (development) = 168 mg/kg/day

(h) STOT-single exposure

No data available

(i) STOT-repeated exposure

No data available

(j) aspiration hazard

No data available

## 12 ECOLOGICAL INFORMATION

### 12.1 Toxicity

Alga, Growth Inhibition Test (Pseudokirchneriella subcapitata, OECD 201):

72 ErC50 = 3.4 mg/l (Based on nominal concentrations)

72 ErC10 = 1.7 mg/l (Based on nominal concentrations)

Daphnia sp. Acute Immobilisation Test (OECD 202, Static): 48 EC50 = 1.7 mg/l (Based on nominal concentrations)

QSAR - Fish, Acute Toxicity Test ( ECOSAR): 96 LC50 = 1.904 mg/l

Data on analogue - Activated Sludge, Respiration Inhibition Test (OECD 209, WAF): 3h EC50 = 960 mg/l (Estimated)

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### 12.2 Persistence and degradability

Ready Biodegradation - Manometric Respirometry Test (301F Screening): (60% in 28 day(s)) (10-day window criterion not fulfilled)

Ready Biodegradation - Modified MITI Test (OECD 301C, Sludge): Non readily biodegradable (19% in 28 day(s))

Stability as a function of pH: Stable but unstable in basic conditions (40°C)

### 12.3 Bioaccumulative potential

Log Kow = 4.1 (OECD 117)

### 12.4 Mobility in soil

Adsorption coefficient: Log Koc = 2.88 - 3.39

### 12.5 Results of PBT and vPvB assessment

Not applicable

### 12.6 Other adverse effects

No data available

## **13 DISPOSAL CONSIDERATIONS**

### **13.1 Waste treatment methods**

Product: The product should be handled according to the instructions given under sections 6, 7 and 8. Dispose of according to local or national regulations. The product should not be allowed to enter drains or the environment

Contaminated packaging: Empty packaging should be disposed according to local or national regulations by an approved waste handling

## **14 TRANSPORT INFORMATION**

In case of accidental spillage or fire during transport, refer to instructions given under points 5, 6, 7 and 8 above.

### UNO

|                             |  |
|-----------------------------|--|
| 14.1 UN-No:                 | 3082   |
| 14.2 Proper Shipping Name:  | Environmentally hazardous substance, liquid, n.o.s. (DIMETHYL-CYCLOHEXENE-PENTENONE) |
| 14.3 Class:                 | 9  |
| 14.4 Packing Group:         | III  |
| 14.5 Environmental hazards: | Yes  |

### Land transport (ADR/RID)

|                            |  |
|----------------------------|--|
| 14.1 UN-No:                | 3082   |
| 14.2 Proper Shipping Name: | ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (DIMETHYL-CYCLOHEXENE-PENTENONE) |
| 14.3 Class:                | 9  |



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14.4 Packing Group: III  
14.5 Environmental hazards: Yes  
14.6 Special precautions for user: Refer to section 7

### Sea transport (IMDG-Code)

14.1 UN-No: 3082  
14.2 Proper Shipping Name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (DIMETHYL-CYCLOHEXENE-PENTENONE)  
14.3 Class: 9  
14.4 Packing Group: III  
14.5 Environmental hazards: Yes  
Marine pollutant: Yes  
14.6 Special precautions for user: Refer to section 7  
14.7 Maritime transport in bulk according to IMO instruments: Not applicable

### Air transport (ICAO-IATA)

14.1 UN-No: 3082  
14.2 Proper Shipping Name: Environmentally hazardous substance, liquid, n.o.s. (DIMETHYL-CYCLOHEXENE-PENTENONE)  
14.3 Class: 9  
14.4 Packing Group: III  
14.5 Environmental hazards: Not applicable  
14.6 Special precautions for user: Refer to section 7  
14.7 Maritime transport in bulk according to IMO instruments: Not applicable

## **15 REGULATORY INFORMATION**

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

No relevant information available at this time.

### 15.2 Chemical Safety Assessment

No data available at this time.

## **16 OTHER INFORMATION**

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### 16.1 Revisions

March-2023 : Version 12 - Updates to sections 1, 2, 3 ,8 ,9, 11, 12, 14, 15, 16

### 16.2 Key literature references

RIFM database  
OECD SIDS  
EU IUCLID  
Supplier information

### 16.3 Full text of phrases used under section 2

|           |  |
|-----------|--|
| H317      | May cause an allergic skin reaction.                                       |
| H303      | May be harmful if swallowed.   |
| H411      | Toxic to aquatic life with long lasting effects.                           |
| P261      | Avoid breathing dust/fume/gas/mist/vapours/spray.                          |
| P273      | Avoid release to the environment.  |
| P272      | Contaminated work clothing should not be allowed out of the workplace.     |
| P280      | Wear protective gloves/protective clothing/eye protection/face protection. |
| P302+P352 | IF ON SKIN: Wash with plenty of soap and water.                            |
| P333+P313 | If skin irritation or rash occurs: Get medical advice/attention.           |
| P391      | Collect spillage.  |
| P312      | Call a POISON CENTER or doctor/physician if you feel unwell.               |
| P363      | Wash contaminated clothing before reuse.                                   |

### 16.4 Full text of phrases used under section 3

|      |  |
|------|--|
| H303 | May be harmful if swallowed.                     |
| H317 | May cause an allergic skin reaction.             |
| H401 | Toxic to aquatic life.                           |
| H411 | Toxic to aquatic life with long lasting effects. |

**We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use of the product are not within the control of Firmenich, it is the user's obligation to determine conditions of safe use of the product.**

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