

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**Trade name **3,6-Dimethyl-4-octyn-3,6-diol**

Stock number: B22491

CAS Number:

78-66-0

EC number:

201-131-8

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

Identified use: SU24 Scientific research and development

**1.3 Details of the supplier of the safety data sheet****Manufacturer/Supplier:**

Thermo Fisher (Kandel) GmbH

Zeppelinstr. 7b

76185 Karlsruhe / Germany

Tel: +49 (0) 721 84007 280

Fax: +49 (0) 721 84007 300

Email: tech@alfa.com

www.alfa.com

Informing department: Product safety Tel + +049 (0) 7275 988687-0

**1.4 Emergency telephone number:**

Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)

Poison Information Center Mainz

www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2 H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

**Classification according to Directive 67/548/EEC or Directive 1999/45/EC**

Xn; Harmful

R22: Harmful if swallowed.

Xi; Irritant

R36/37/38: Irritating to eyes, respiratory system and skin.

**Information concerning particular hazards for human and environment:** Not applicable**Other hazards that do not result in classification** No information known.**2.2 Label elements****Labelling according to Regulation (EC) No 1272/2008** The substance is classified and labelled according to the CLP regulation.**Hazard pictograms**

GHS07

**Signal word** Warning**Hazard statements**

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

**Precautionary statements**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

**2.3 Other hazards****Results of PBT and vPvB assessment****PBT:** Not applicable.**vPvB:** Not applicable.**SECTION 3: Composition/information on ingredients****3.1 Substances****CAS# Designation:**

78-66-0 3,6-Dimethyl-4-octyn-3,6-diol

**Identification number(s):**

EC number: 201-131-8

**SECTION 4: First aid measures****4.1 Description of first aid measures****After inhalation**

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

Seek immediate medical advice.

**After skin contact**

Instantly wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

**After eye contact** Rinse opened eye for several minutes under running water. Then consult doctor.**After swallowing** Seek medical treatment.**4.2 Most important symptoms and effects, both acute and delayed** No further relevant information available.**4.3 Indication of any immediate medical attention and special treatment needed** No further relevant information available.

Trade name **3,6-Dimethyl-4-octyn-3,6-diol**

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### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

**Suitable extinguishing agents** CO<sub>2</sub>, extinguishing powder or water jet. Fight larger fires with water jet or alcohol-resistant foam.

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

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

#### 5.3 Advice for firefighters

##### Protective equipment:

Wear self-contained breathing apparatus.

Wear full protective suit.

### SECTION 6: Accidental release measures

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

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

**6.2 Environmental precautions:** Do not allow material to be released to the environment without proper governmental permits.

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

Dispose of contaminated material as waste according to section 13.

Ensure adequate ventilation.

**Prevention of secondary hazards:** No special measures required.

#### 6.4 Reference to other sections

See Section 7 for information on safe handling

See section 8 for information on personal protection equipment.

See Section 13 for information on disposal.

### SECTION 7: Handling and storage

#### 7.1 Precautions for safe handling

Keep containers tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation/exhaustion at the workplace.

**Information about protection against explosions and fires:** No information known.

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

##### Storage

**Requirements to be met by storerooms and containers:** No special requirements.

**Information about storage in one common storage facility:** Store away from oxidising agents.

##### Further information about storage conditions:

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

**7.3 Specific end use(s)** No further relevant information available.

### SECTION 8: Exposure controls/personal protection

#### Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

#### 8.1 Control parameters

**Components with critical values that require monitoring at the workplace:** Not required.

**Additional information:** No data

#### 8.2 Exposure controls

##### Personal protective equipment

##### General protective and hygienic measures

The usual precautionary measures should be adhered to in handling the chemicals.

Keep away from foodstuffs, beverages and food.

Instantly remove any soiled and impregnated garments.

Wash hands during breaks and at the end of the work.

Avoid contact with the eyes and skin.

Maintain an ergonomically appropriate working environment.

**Breathing equipment:** Use breathing protection with high concentrations.

##### Protection of hands:

Check protective gloves prior to each use for their proper condition.

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

**Material of gloves** Impervious gloves

**Penetration time of glove material (in minutes)** Not determined

##### Eye protection:

Safety glasses

Face protection

**Body protection:** Protective work clothing.

### SECTION 9: Physical and chemical properties

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

##### General Information

##### Appearance:

<b>Form:</b>	Powder
<b>Colour:</b>	Off-white
<b>Smell:</b>	Not determined
<b>Odour threshold:</b>	Not determined.

<b>pH-value:</b>	Not applicable.
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##### Change in condition

<b>Melting point/Melting range:</b>	53-55 °C
<b>Boiling point/Boiling range:</b>	208-214 °C (680 mmHg)
<b>Sublimation temperature / start:</b>	Not determined

<b>Flash point:</b>	Not applicable
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<b>Inflammability (solid, gaseous)</b>	Not determined.
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<b>Ignition temperature:</b>	Not determined
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<b>Decomposition temperature:</b>	Not determined
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<b>Self-inflammability:</b>	Not determined.
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<b>Danger of explosion:</b>	Product is not explosive.
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##### Critical values for explosion:

<b>Lower:</b>	Not determined
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<b>Upper:</b>	Not determined
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<b>Steam pressure:</b>	Not applicable.
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<b>Density</b>	Not determined
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<b>Relative density</b>	Not determined.
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<b>Vapour density</b>	Not applicable.
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Trade name **3,6-Dimethyl-4-octyn-3,6-diol**

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**Evaporation rate** Not applicable.  
**Solubility in / Miscibility with Water:** Not determined  
**Partition coefficient (n-octanol/water):** Not determined.  
**Viscosity:**  
**dynamic:** Not applicable.  
**kinematic:** Not applicable.  
**9.2 Other information** No further relevant information available.

### SECTION 10: Stability and reactivity

**10.1 Reactivity** No information known.  
**10.2 Chemical stability** Stable under recommended storage conditions.  
**Thermal decomposition / conditions to be avoided:** No decomposition if used and stored according to specifications.  
**10.3 Possibility of hazardous reactions** No dangerous reactions known  
**10.4 Conditions to avoid** No further relevant information available.  
**10.5 Incompatible materials:** Oxidising agents  
**10.6 Hazardous decomposition products:** Carbon monoxide and carbon dioxide

### SECTION 11: Toxicological information

**11.1 Information on toxicological effects**  
**Acute toxicity:** Harmful if swallowed.  
**LD/LC50 values that are relevant for classification:** No data  
**Skin irritation or corrosion:** Causes skin irritation.  
**Eye irritation or corrosion:** Causes serious eye irritation.  
**Sensitization:** No sensitizing effect known.  
**Germ cell mutagenicity:** No effects known.  
**Carcinogenicity:** No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.  
**Reproductive toxicity:** No effects known.  
**Specific target organ system toxicity - repeated exposure:** No effects known.  
**Specific target organ system toxicity - single exposure:** May cause respiratory irritation.  
**Aspiration hazard:** No effects known.  
**Subacute to chronic toxicity:** No effects known.  
**Additional toxicological information:** To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

### SECTION 12: Ecological information

**12.1 Toxicity**  
**Aquatic toxicity:** No further relevant information available.  
**12.2 Persistence and degradability** No further relevant information available.  
**12.3 Bioaccumulative potential** No further relevant information available.  
**12.4 Mobility in soil** No further relevant information available.  
**Additional ecological information:**  
**General notes:**  
Do not allow material to be released to the environment without proper governmental permits.  
Water hazard class 1 (Self-assessment): slightly hazardous for water.  
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.  
Avoid transfer into the environment.  
**12.5 Results of PBT and vPvB assessment**  
**PBT:** Not applicable.  
**vPvB:** Not applicable.  
**12.6 Other adverse effects** No further relevant information available.

### SECTION 13: Disposal considerations

**13.1 Waste treatment methods**  
**Recommendation**  
Hand over to disposers of hazardous waste.  
Must be specially treated under adherence to official regulations.  
Consult state, local or national regulations for proper disposal.  
**Uncleaned packagings:**  
**Recommendation:** Disposal must be made according to official regulations.

### SECTION 14: Transport information

<b>UN-Number</b> <b>ADR, IMDG, IATA</b>	None
<b>14.2 UN proper shipping name</b> <b>ADR, IMDG, IATA</b>	None
<b>14.3 Transport hazard class(es)</b> <b>ADR, IMDG, IATA</b> <b>Class</b>	None
<b>Packing group</b> <b>ADR, IMDG, IATA</b>	None
<b>14.5 Environmental hazards:</b>	Not applicable.
<b>14.6 Special precautions for user</b>	Not applicable.
<b>14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	Not applicable.
<b>Transport/Additional information:</b>	Not dangerous according to the above specifications.

### SECTION 15: Regulatory information

**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**  
**Australian Inventory of Chemical Substances** Substance is listed.  
**Standard for the Uniform Scheduling of Drugs and Poisons** Substance is not listed.  
**National regulations**  
**Information about limitation of use:**  
Employment restrictions concerning young persons must be observed.  
For use only by technically qualified individuals.  
**Water hazard class:** Water hazard class 1 (Self-assessment): slightly hazardous for water.  
**Other regulations, limitations and prohibitive regulations**  
**ELINCS (European List of Notified Chemical Substances)** Substance is not listed.

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Trade name **3,6-Dimethyl-4-octyn-3,6-diol**

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**Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006.** Substance is not listed.  
**The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.**  
Substance is not listed.  
**Annex XIV of the REACH Regulations (requiring Authorisation for use)** Substance is not listed.  
**15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

**SECTION 16: Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

**Department issuing SDS:** Global Marketing Department

**Abbreviations and acronyms:**

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)  
IMDG: International Maritime Code for Dangerous Goods  
IATA: International Air Transport Association  
GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
EINECS: European Inventory of Existing Commercial Chemical Substances  
CAS: Chemical Abstracts Service (division of the American Chemical Society)  
LC50: Lethal concentration, 50 percent  
LD50: Lethal dose, 50 percent  
vPvB: very Persistent and very Bioaccumulative  
ACGIH: American Conference of Governmental Industrial Hygienists (USA)  
OSHA: Occupational Safety and Health Administration (USA)  
NTP: National Toxicology Program (USA)  
IARC: International Agency for Research on Cancer  
EPA: Environmental Protection Agency (USA)

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