

Creation Date 26-Sep-2009

Revision Date 29-Sep-2023

Revision Number 5

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: **1,6-Heptadiyne**
Cat No. : **309420000; 309420010; 309420050**
CAS No **2396-63-6**
Molecular Formula **C7 H8**

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

Recommended Use Laboratory chemicals.
Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

EU entity/business name
Thermo Fisher Scientific
Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

UK entity/business name
Fisher Scientific UK
Bishop Meadow Road,
Loughborough, Leicestershire LE11 5RG, United Kingdom

Swiss distributor - Fisher Scientific AG
Neuhofstrasse 11, CH 4153 Reinach
Tel: +41 (0) 56 618 41 11
e-mail - infoch@thermofisher.com

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

customers in Switzerland:
Tox Info Suisse Emergency Number: **145 (24hr)**
Tox Info Suisse: +41-44 251 51 51 (Emergency number from abroad)
Chemtrec (24h) Toll-Free: 0800 564 402
Chemtrec Local: +41-43 508 20 11 (Zurich)

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

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CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

Flammable liquids

Category 2 (H225)

Health hazards

Based on available data, the classification criteria are not met

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Danger

Hazard Statements

H225 - Highly flammable liquid and vapor

Precautionary Statements

P240 - Ground and bond container and receiving equipment

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - Regulation (EC) No 1272/2008 |
|----------------|-----------|-------------------|----------|---|
| 1,6-Heptadiyne | 2396-63-6 | EEC No. 219-253-5 | 98 | Flam. Liq. 2 (H225) |

Full text of Hazard Statements: see section 16

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SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

| | |
|---|--|
| Eye Contact | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention. |
| Skin Contact | Wash off immediately with plenty of water for at least 15 minutes. Get medical attention. |
| Ingestion | Do NOT induce vomiting. Get medical attention. |
| Inhalation | Remove to fresh air. If not breathing, give artificial respiration. Get medical attention. |
| Self-Protection of the First Aider | Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination. |

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

Difficulty in breathing. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician Treat symptomatically. Symptoms may be delayed.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Flammable. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

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Prevent further leakage or spillage if safe to do so.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Ensure adequate ventilation. Wear personal protective equipment/face protection. Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Keep away from open flames, hot surfaces and sources of ignition. Wash hands before breaks and immediately after handling the product. Take precautionary measures against static discharges. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep refrigerated. Flammables area. Keep container tightly closed in a dry and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510
Storage Class (LGK) (Germany)

Class 3

Switzerland - Storage of hazardous substances

Storage class - SC 3
<https://www.kvu.ch/de/themen/stoffe-und-produkte>
<https://www.kvu.ch/fr/themes/substances-et-produits>
<https://www.kvu.ch/it/temi/sostanze-e-prodotti>

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

| Component | European Union | The United Kingdom | France | Belgium | Spain |
|----------------|----------------|--------------------|--|---------|-------|
| 1,6-Heptadiyne | | | TWA / VME: 1000 mg/m ³ (8 heures). STEL / VLCT: 1500 mg/m ³ . | | |

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Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection

Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments |
|-----------------------------|--------------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber Viton (R) | See manufacturers recommendations | - | EN 374 | (minimum requirement) |

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use. observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information) gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. gloves with care avoiding skin contamination.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

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Small scale/Laboratory use Maintain adequate ventilation

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

| | | |
|---|--------------------------|-----------------------------------|
| Physical State | Liquid | |
| Appearance | Light yellow | |
| Odor | No information available | |
| Odor Threshold | No data available | |
| Melting Point/Range | -85 °C / -121 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 111.5 °C / 232.7 °F | |
| Flammability (liquid) | Highly flammable | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Flash Point | 9 °C / 48.2 °F | Method - No information available |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | No data available | |
| Water Solubility | Insoluble | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Vapor Pressure | No data available | |
| Density / Specific Gravity | 0.805 | |
| Bulk Density | Not applicable | Liquid |
| Vapor Density | No data available | (Air = 1.0) |
| Particle characteristics | (liquid) Not applicable | |

9.2. Other information

| | |
|----------------------|---|
| Molecular Formula | C7 H8 |
| Molecular Weight | 92.15 |
| Explosive Properties | Vapors may form explosive mixtures with air |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions No information available.

10.4. Conditions to avoid Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

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10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information No acute toxicity information is available for this product

(a) acute toxicity;

Oral

Based on available data, the classification criteria are not met

Dermal

No data available

Inhalation

No data available

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|----------------|---------------------------|-------------|-----------------|
| 1,6-Heptadiyne | LD50 = 2300 mg/kg (Rat) | - | - |

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory

No data available

Skin

No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs

No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting.

11.2. Information on other hazards

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Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

12.2. Persistence and degradability

Persistence

Insoluble in water, Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

May have some potential to bioaccumulate

12.4. Mobility in soil

Spillage unlikely to penetrate soil The product is insoluble and floats on water The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Is not likely mobile in the environment due its low water solubility. Will likely be mobile in the environment due to its volatility.

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects **Persistent Organic Pollutant** **Ozone Depletion Potential**

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

Switzerland - Waste Ordinance

Disposal should be in accordance with applicable regional, national and local laws and

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regulations. Ordinance on the Avoidance and the Disposal of Waste (Waste Ordinance, ADWO) SR 814.600
<https://www.fedlex.admin.ch/eli/cc/2015/891/en>

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN1993
14.2. UN proper shipping name Flammable liquid, n.o.s.
Technical Shipping Name 1,6-Heptadiyne
14.3. Transport hazard class(es) 3
14.4. Packing group II

ADR

14.1. UN number UN1993
14.2. UN proper shipping name Flammable liquid, n.o.s.
Technical Shipping Name 1,6-Heptadiyne
14.3. Transport hazard class(es) 3
14.4. Packing group II

IATA

14.1. UN number UN1993
14.2. UN proper shipping name FLAMMABLE LIQUID, N.O.S.*
Technical Shipping Name 1,6-Heptadiyne
14.3. Transport hazard class(es) 3
14.4. Packing group II

14.5. Environmental hazards No hazards identified
14.6. Special precautions for user No special precautions required.
14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component | CAS No | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|----------------|-----------|-----------|--------|-----|-------|------|------|------|------|
| 1,6-Heptadiyne | 2396-63-6 | 219-253-5 | - | - | - | X | - | - | - |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDL | AICS | NZIoC | PICCS |
|----------------|-----------|------|---|-----|-----|------|-------|-------|
| 1,6-Heptadiyne | 2396-63-6 | X | ACTIVE | - | X | - | - | - |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Not applicable

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| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|----------------|-----------|---|---|---|
| 1,6-Heptadiyne | 2396-63-6 | - | - | - |

Seveso III Directive (2012/18/EC)

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|----------------|-----------|---|--|
| 1,6-Heptadiyne | 2396-63-6 | Not applicable | Not applicable |

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 2 (self classification)

Swiss Regulations

Article 4 para. 4 of the Ordinance on the protection of young people in the workplace (SR 822.115) and Article 1 lit. f of the EAER regulation on hazardous work and young people (SR 822.115.2).

Take note on Article 13 Maternity Ordinance (SR 822.111.52) with regards expectant and nursing mothers.

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

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

H225 - Highly flammable liquid and vapor

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

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WEL - Workplace Exposure Limit
ACGIH - American Conference of Governmental Industrial Hygienists
DNEL - Derived No Effect Level
RPE - Respiratory Protective Equipment
LC50 - Lethal Concentration 50%
NOEC - No Observed Effect Concentration
PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average
IARC - International Agency for Research on Cancer
Predicted No Effect Concentration (PNEC)
LD50 - Lethal Dose 50%
EC50 - Effective Concentration 50%
POW - Partition coefficient Octanol:Water
vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code
OECD - Organisation for Economic Co-operation and Development
BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
MARPOL - International Convention for the Prevention of Pollution from Ships
ATE - Acute Toxicity Estimate
VOC - (volatile organic compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>
Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

Chemical incident response training.

Creation Date 26-Sep-2009
Revision Date 29-Sep-2023
Revision Summary Not applicable.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No 1907/2006 .

For Switzerland - Compiled in accordance with the technical provisions referred to in Annex 2, Number 3, ChemO (SR 813.11 - Ordinance on Protection against Dangerous Substances and Preparations).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet