

Creation Date 18-Oct-2010

Revision Date 27-Jan-2024

Revision Number 3

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

### 1.1. Product identifier

Product Description: **1-Heptyne**  
 Cat No. : **A11130**  
 CAS No **628-71-7**  
 Molecular Formula **C7 H12**  
 REACH registration number **-**

### 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 Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
 Shore Road, Heysham  
 Lancashire, LA3 2XY,  
 United Kingdom  
 Office Tel: +44 (0) 1524 850506  
 Office Fax: +44 (0) 1524 850608

E-mail address [bege1.sdsdesk@thermofisher.com](mailto:bege1.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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Flammable liquids Category 2 (H225)

##### Health hazards

Aspiration Toxicity Category 1 (H304)

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation  
Specific target organ toxicity - (single exposure)

Category 2 (H315)  
Category 2 (H319)  
Category 3 (H335)

## **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  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

## **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  
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
P331 - Do NOT induce vomiting  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
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

## **2.3. Other hazards**

Toxic to terrestrial vertebrates  
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 - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
1-Heptyne	628-71-7	EEC No. 211-051-5	>95	Flam. Liq. 2 (H225) STOT SE 3 (H335) Asp. Tox. 1 (H304) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

REACH registration number

-

Full text of Hazard Statements: see section 16

## SECTION 4: FIRST AID MEASURES

### 4.1. Description of first aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
<b>Inhalation</b>	Remove to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Get medical attention. Risk of serious damage to the lungs (by aspiration).
<b>Self-Protection of the First Aider</b>	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.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

#### **Extinguishing media which must not be used for safety reasons**

No information available.

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

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

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

### 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. Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 6: ACCIDENTAL RELEASE MEASURES

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

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

Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

## 6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

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

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

## 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

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. 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 containers tightly closed in a dry, cool and well-ventilated place. Flammables area. Keep away from heat, sparks and flame.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 3  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

List source(s):

#### **Biological limit values**

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

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

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

No information available

## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. 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) Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, 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.

Remove 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

**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

<b>Physical State</b>	Liquid
<b>Appearance</b>	Colorless to Yellow-Green
<b>Odor</b>	No information available
<b>Odor Threshold</b>	No data available
<b>Melting Point/Range</b>	-81 °C / -113.8 °F
<b>Softening Point</b>	No data available
<b>Boiling Point/Range</b>	99 - 100 °C / 210.2 - 212 °F @ 760 mmHg

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

<b>Flammability (liquid)</b>	Highly flammable	On basis of test data
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	-2 °C / 28.4 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	No data available	
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	93.1 mmHg @ 37.7 °C	
<b>Density / Specific Gravity</b>	0.730	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

## 9.2. Other information

<b>Molecular Formula</b>	C7 H12
<b>Molecular Weight</b>	96.17
<b>Explosive Properties</b>	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

<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

### 10.4. Conditions to avoid

Incompatible products. Excess heat. Keep away from open flames, hot surfaces and sources of ignition.

### 10.5. Incompatible materials

Strong oxidizing agents. Halogenated compounds. Metals.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

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

<b>Product Information</b>	No acute toxicity information is available for this product
<b>(a) acute toxicity;</b>	
<b>Oral</b>	No data available
<b>Dermal</b>	No data available
<b>Inhalation</b>	No data available

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(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;	Category 3
Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	Category 1
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

**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** Do not empty into drains.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB assessment No data available for assessment.

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

## 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**

This product does not contain any known or suspected substance

### **Ozone Depletion Potential**

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.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

#### 14.1. UN number

UN3295

#### 14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

#### Technical Shipping Name

(1-HEPTYNE)

#### 14.3. Transport hazard class(es)

3

#### 14.4. Packing group

II

### ADR

#### 14.1. UN number

UN3295

#### 14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

#### Technical Shipping Name

(1-HEPTYNE)

#### 14.3. Transport hazard class(es)

3

#### 14.4. Packing group

II

### IATA

#### 14.1. UN number

UN3295

#### 14.2. UN proper shipping name

Hydrocarbons, liquid, n.o.s.

#### Technical Shipping Name

(1-HEPTYNE)

#### 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.



# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

**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/NDSL), 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-Heptyne	628-71-7	211-051-5	-	-	-	X	KE-18373	-	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
1-Heptyne	628-71-7	X	ACTIVE	-	X	X	X	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

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-Heptyne	628-71-7	-	-	-

#### 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-Heptyne	628-71-7	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 = 3 (self classification)

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
1-Heptyne 628-71-7 (>95)	Prohibited and Restricted Substances		

## 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  
H304 - May be fatal if swallowed and enters airways  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

### 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

**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

### Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**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)

### 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.

### Prepared By

Health, Safety and Environmental Department

### Creation Date

18-Oct-2010

### Revision Date

27-Jan-2024

### Revision Summary

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as**

# SAFETY DATA SHEET

1-Heptyne

Revision Date 27-Jan-2024

---

amended. .

## 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**