

according to Regulation (EC) No 1907/2006

### NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 21.06.2024

Product code: 203210

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

### 1.1. Product identifier

NATURAL ALLYL HEXANOATE (CAPROATE)

Substance name:	NATURAL ALLYL HEXANOATE (CAPROATE)
CAS No:	123-68-2
EC No:	204-642-4

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

#### Use of the substance/mixture

For Flavour use for food and feed only

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

Company name:	Axxence Aromatic GmbH	
Street:	Tackenweide 28	
Place:	D-46446 Emmerich am Rhein	
Telephone:	+ 49 2822 68561 0	Telefax: + 49 2822 68561 39
E-mail:	info@axxence.com	
Contact person:	Safety Team	Telephone: + 49 2822 68561 0
E-mail:	safety-documentation@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	Safety Management	
1.4. Emergency telephone	+49 2822 68561 99	

### number:

**SECTION 2: Hazards identification** 

### 2.1. Classification of the substance or mixture

#### Regulation (EC) No 1272/2008 Acute Tox. 3; H311 Acute Tox. 3; H301 Acute Tox. 3; H301

Acute Tox. 3; H301 Aquatic Acute 1; H400 Aquatic Chronic 3; H412

Full text of hazard statements: see SECTION 16.

#### 2.2. Label elements

#### Regulation (EC) No 1272/2008

Signal word:

**Pictograms:** 



### Hazard statements

H301+H311 H410	Toxic if swallowed or in contact with skin. Very toxic to aquatic life with long lasting effects.
Precautionary statem	ents
P264	Wash hands thoroughly after handling.

P264	Wash hands thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing
	protection.
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.



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P321	Specific treatment (see on this label).	
P330	Rinse mouth.	
P302+P352	IF ON SKIN: Wash with plenty of water.	
P312	Call a POISON CENTER/doctor if you feel unwell.	
P321	Specific treatment (see on this label).	
P361+P364	Take off immediately all contaminated clothing and wash it before reuse.	
P391	Collect spillage.	
P405	Store locked up.	
P501	Dispose of contents/container to organic waste.	

### 2.3. Other hazards

This substance is not listed as Substance of Very High Concern (SVHC) in the Candidate List according to REACH, Article 59. This substance is not identifed as SVHC (substance of very high concern) and is not subject to autorisation according to Annex XIV of REACH.

### **SECTION 3: Composition/information on ingredients**

#### 3.1. Substances

Sum formula:	C9 H16 O2
Molecular weight:	156,22 g/mol

### **Relevant ingredients**

CAS No	Chemical name			Quantity		
	EC No	EC No Index No REACH No				
	Classification (Regulation (EC) No 1272/2008)					
123-68-2	NATURAL ALLYL HEXANOATE (C	NATURAL ALLYL HEXANOATE (CAPROATE)				
	204-642-4					
	Acute Tox. 3, Acute Tox. 3, Aquatic Acute 1, Aquatic Chronic 3; H311 H301 H400 H412					

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		
123-68-2	204-642-4 NATURAL ALLYL HEXANOATE (CAPROATE)		100 %
	dermal: LD50 = 820 mg/kg; oral: LD50 = 218 mg/kg		

### SECTION 4: First aid measures

### 4.1. Description of first aid measures

### **General information**

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down.

### After inhalation

Provide fresh air. Medical treatment necessary.

#### After contact with skin

After contact with skin, wash immediately with plenty of water and soap. Take off immediately all contaminated clothing and wash it before reuse. Call a physician immediately.

#### After contact with eyes

After eye contact: Rinse immediately carefully and thoroughly with eye-bath or water. Consult an ophthalmologist.

### After ingestion

Observe risk of aspiration if vomiting occurs. Rinse mouth immediately and drink 1 glass of of water. Induce vomiting when the affected person is not unconscious. Call a physician immediately.



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

No information available.

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

Treat symptomatically.

#### **SECTION 5: Firefighting measures**

#### 5.1. Extinguishing media

#### Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings.

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

Non-flammable. Vapours can form explosive mixtures with air. Heating causes rise in pressure with risk of bursting.

#### 5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

### Additional information

Use water spray jet to protect personnel and to cool endangered containers. Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

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

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

### General advice

Provide adequate ventilation.

#### For emergency responders

Suppress gases/vapours/mists with water spray jet. Wear a self-contained breathing apparatus and chemical protective clothing.

#### 6.2. Environmental precautions

Do not allow uncontrolled discharge of product into the environment.

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

### For cleaning up

Ventilate affected area.

#### Other information

Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents). Treat the recovered material as prescribed in the section on waste disposal.

### 6.4. Reference to other sections

Safe handling: see section 7 Personal protection equipment: see section 8 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 have to be used. Do not breathe gas/fumes/vapour/spray.

### Advice on protection against fire and explosion

No special fire protection measures are necessary.

#### Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.

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Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme. Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff.

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

#### Requirements for storage rooms and vessels

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaustion at critical locations.

#### Hints on joint storage

No special measures are necessary.

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

For Flavour use for food and feed only

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

#### 8.1. Control parameters

### DNEL/DMEL values

CAS No	Name of agent				
DNEL type	type Exposure route Effect Value				
123-68-2 NATURAL ALLYL HEXANOATE (CAPROATE)					
Worker DNEL,	long-term	inhalation	systemic	15 mg/m³	
Worker DNEL,	EL, long-term dermal systemic 4,3 mg/kg bw/day				
Consumer DNE	onsumer DNEL, long-term inhalation systemic 3,7 mg/m <sup>3</sup>				
Consumer DNEL, long-term dermal systemic 2,1 mg/kg bw/day					
Consumer DNEL, long-term oral systemic 2,1 mg/kg bw/da				2,1 mg/kg bw/day	

### **PNEC** values

CAS No	Name of agent				
Environmental	Environmental compartment Value				
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)				
Freshwater	Freshwater 0,00012 mg/l				
Marine water	ter 0,000012 mg/l				
Freshwater sediment 0,00446 mg/kg					
Marine sediment 0,000446 mg/kg					
Micro-organisms in sewage treatment plants (STP) 10 mg/l					
Soil 0,000825 mg/kg					

#### 8.2. Exposure controls



### Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

Individual protection measures, such as personal protective equipment

#### Eye/face protection

Wear eye protection/face protection.



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#### Hand protection

Suitable gloves type: NBR (Nitrile rubber) + Natural fibres (e.g. cotton) When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. 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. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Suitable gloves type NBR (Nitrile rubber) + Natural fibres (e.g. cotton)

### Skin protection

Use of protective clothing.

### **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: Melting point/freezing Boiling point or initial		<-20 °C 187 °C
boiling range: Flammability: Lower explosion limit	s:	not determined not determined
Upper explosion limit	s:	not determined
Flash point: Auto-ignition tempera		63 °C 268 °C
Decomposition tempe	erature:	not determined
pH-Value:		not determined
Viscosity / kinematic: (at 20 °C)		1,22 mm²/s
Water solubility:		0,41 g/l
(at 20 °C)		
Solubility in other solv	vents	
not determined		
Partition coefficient n Vapour pressure:	-octanol/water:	3,2 2,69 hPa
(at 20 °C)		2,09 m a
Density (at 20 °C):		0,89 g/cm <sup>3</sup>
Relative vapour dens	ity:	5,39
(at 20 °C)		
Particle characteristic	CS:	not applicable
9.2. Other information		
-	ard to physical hazard classes	
Explosive properties	to Eveloping and eveloping approximate EUA 44	
Oxidizing properties	t: Explosive. not explosive according to EU A.14	
The product is no	t: oxidisina.	
Other safety charact		
Evaporation rate:		not determined
Solvent content:		0%
Solid content:		0%
Viscosity / dynamic:		1,09 mPa·s
(at 20 °C)		



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### **SECTION 10: Stability and reactivity**

#### 10.1. Reactivity

No hazardous reaction when handled and stored according to provisions.

### 10.2. Chemical stability

The product is stable under storage at normal ambient temperatures.

#### 10.3. Possibility of hazardous reactions

No known hazardous reactions.

#### 10.4. Conditions to avoid

none

### 10.5. Incompatible materials

No information available.

#### 10.6. Hazardous decomposition products

No known hazardous decomposition products.

#### **SECTION 11: Toxicological information**

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

#### Acute toxicity

Toxic if swallowed.

Toxic in contact with skin.

CAS No	Chemical name						
	Exposure route Dose Species Source Method						
123-68-2	NATURAL ALLYL HEXA	NATURAL ALLYL HEXANOATE (CAPROATE)					
	oral	LD50 mg/kg	218	Rat	REACH Dossier	OECD 401	
	dermal	LD50 mg/kg	820	Rabbit	REACH Dossier	OECD 402	

#### Irritation and corrosivity

Skin corrosion/irritation: Based on available data, the classification criteria are not met. Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

#### Sensitising effects

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

### Carcinogenic/mutagenic/toxic effects for reproduction

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

#### STOT-single exposure

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

### 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.

#### 11.2. Information on other hazards

#### Endocrine disrupting properties

No information available.

#### **SECTION 12: Ecological information**



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### 12.1. Toxicity

Very toxic to aquatic life.

Harmful to aquatic life with long lasting effects.

Very toxic to aquatic life. Harmful to aquatic life with long lasting effects.

CAS No	Chemical name							
	Aquatic toxicity	Dose		[h]   [d]	Species	Source	Method	
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)							
	Acute fish toxicity	LC50 mg/l	0,117	96 h	Danio rerio (zebrafish)	REACH Registration	OEDC 203	
	Acute algae toxicity	ErC50 mg/l	>4,6		Desmodesmus subspicatus	REACH Registration	OECD 201	
	Acute crustacea toxicity	EC50	2,0 mg/l		Daphnia magna (Big water flea)	REACH Registration	OECD TG 202	
	Algae toxicity	NOEC mg/l	0,158		Desmodesmus subspicatus	REACH Registration	OECD 201	

### 12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name						
	Method	Value		d	Source		
	Evaluation		=				
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)						
	OECD 301F	19%		2	REACH Registration		
	Readily biodegradable (according to OECD criteria).						
	OECD 301F	62%		7	REACH Registration		
	Readily biodegradable (according to OECD criteria).						
	OECD 301F	70%		28	REACH Registration		
	Readily biodegradable (according to OECD criteria).						

#### 12.3. Bioaccumulative potential

The product has not been tested.

### Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	3,191

### BCF

CAS No	Chemical name	BCF	Species	Source
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	102,3	Fish	REACH Registration

#### 12.4. Mobility in soil

The product has not been tested.

### 12.5. Results of PBT and vPvB assessment

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

The product has not been tested.

### 12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms. No information available.

### 12.7. Other adverse effects

No information available.

### **Further information**

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



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### **SECTION 13: Disposal considerations**

#### 13.1. Waste treatment methods

## **Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation.

#### List of Wastes Code - residues/unused products

WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes containing hazardous substances; hazardous waste

#### List of Wastes Code - used product

160305 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes containing hazardous substances; hazardous waste

#### List of Wastes Code - contaminated packaging

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

### Contaminated packaging

Hazardous waste according to Directive 2008/98/EC (waste framework directive). Handle contaminated packages in the same way as the substance itself.

### **SECTION 14: Transport information**

#### Land transport (ADR/RID)

<u>14.1. UN number or ID number:</u>	UN 2810
14.2. UN proper shipping name:	TOXIC LIQUID, ORGANIC, N.O.S.
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	III
Hazard label:	6.1
	6
Classification code:	T1
Special Provisions:	274 614
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	2
Hazard No:	60
Tunnel restriction code:	E
Other applicable information (land transp E1	ort)
Inland waterways transport (ADN)	
<u>14.1. UN number or ID number:</u>	UN 2810
14.2. UN proper shipping name:	TOXIC LIQUID, ORGANIC, N.O.S.
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	III
Hazard label:	6.1
	6
Classification code:	T1



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Special Provisions:	274 614 802					
Limited quantity:	5 L					
Excepted quantity:	E1					
Other applicable information (inland wa	terways transport)					
Marine transport (IMDG)						
14.1. UN number or ID number:	UN 2810					
14.2. UN proper shipping name:	TOXIC LIQUID, ORGANIC, N.O.S.					
14.3. Transport hazard class(es):	6.1					
14.4. Packing group:	III					
Hazard label:	6.1					
	6					
Special Provisions:	223 274					
Limited quantity:	5 L					
Excepted quantity:	E1					
EmS:	F-A, S-A					
Air transport (ICAO-TI/IATA-DGR)						
<u>14.1. UN number or ID number:</u>	UN 2810					
14.2. UN proper shipping name:	TOXIC LIQUID, ORGANIC, N.O.S.					
14.3. Transport hazard class(es):	6.1					
14.4. Packing group:	III					
Hazard label:	6.1					
	6					
Special Provisions:	A3 A4 A137					
Limited quantity Passenger:	2 L					
Passenger LQ:	Y642					
Excepted quantity:	E1					
IATA-packing instructions - Passenger:	655					
IATA-max. quantity - Passenger:	60 L					
IATA-packing instructions - Cargo:	663					
IATA-max. quantity - Cargo:	220 L					
4.5. Environmental hazards						
ENVIRONMENTALLY HAZARDOUS:	Yes	NU				
		$\langle \mathbf{Y}_2 \rangle$				
Danger releasing substance:	ALLYL HEXANOATE					
14.6. Special precautions for user Warning: Acute Toxicity.						
14.7. Maritime transport in bulk according	to IMO instruments					
not applicable						
SECTION 15: Regulatory information						
	ulations/legislation specific for the substance or n					

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

## EU regulatory information

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Directive 2010/75/EU on industrial emissions:	100 % (890 g/l)					
Directive 2004/42/EC on VOC in paints and varnishes:	100 % (890 g/l)					
Information according to Directive 2012/18/EU (SEVESO III):	E1 Hazardous to the Aquatic Environment					
Additional information To follow: 850/2004/EC, 79/117/EEC, 6	689/2008/EC					
National regulatory information						
Employment restrictions:	Observe restrictions to employment for juveniles according to the work protection guideline' (94/33/EC). Observe employment rest under the Maternity Protection Directive (92/85/EEC) for expecta nursing mothers.	rictions				
Water hazard class (D):	2 - obviously hazardous to water					
Skin resorption/Sensitization:	Permeates easily through outer skin and causes poisoning.					
15.2. Chemical safety assessment						

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

## **SECTION 16: Other information**

### Changes

This data sheet contains changes from the previous version in section(s): 2.



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### Abbreviations and acronyms

Acute Tox: Acute toxicity Aquatic Acute: Acute aquatic hazard Aquatic Chronic: Chronic aquatic hazard 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 ELINCS: European List of Notified Chemical Substances CAS: Chemical Abstracts Service LC50: Lethal concentration. 50% LD50: Lethal dose, 50% CLP: Classification, labelling and Packaging REACH: Registration, Evaluation and Authorization of Chemicals GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals UN: United Nations DNFL: Derived No Effect Level DMEL: Derived Minimal Effect Level PNEC: Predicted No Effect Concentration ATE: Acute toxicity estimate LL50: Lethal loading, 50% EL50: Effect loading, 50% EC50: Effective Concentration 50% ErC50: Effective Concentration 50%, growth rate NOEC: No Observed Effect Concentration BCF: Bio-concentration factor PBT: persistent, bioaccumulative, toxic vPvB: very persistent, very bioaccumulative RID: Regulations concerning the international carriage of dangerous goods by rail ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures) EmS: Emergency Schedules MFAG: Medical First Aid Guide ICAO: International Civil Aviation Organization MARPOL: International Convention for the Prevention of Marine Pollution from Ships IBC: Intermediate Bulk Container VOC: Volatile Organic Compounds SVHC: Substance of Very High Concern For abbreviations and acronyms, see table at http://abbrev.esdscom.eu For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety assessment, chapter R.20 (Table of terms and abbreviations). EC/EEC: European Community/European Economic Community EU: European Union M-factor: Multiplying factor IATA: International Air Transport Association DGR: Dangerous Goods Regulations ICAO: International Civil Aviation Organization **TI: Technical Instructions** VOC: volatile organic compound Relevant H and EUH statements (number and full text)

## H301 Toxic if swallowed

11301	
H301+H311	Toxic if swallowed or in contact with skin.

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H311Toxic in contact with skin.H400Very toxic to aquatic life.H410Very toxic to aquatic life with long lasting effects.

H412 Harmful to aquatic life with long lasting effects.

### **Further Information**

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

#### Identified uses

No	Short title	LCS	SU	PC	PROC	ERC	AC	TF	Specification
	For Flavour use for food and feed only	-	-	-	-	-	-	-	Flavour

LCS: Life cycle stages

PC: Product categories

ERC: Environmental release categories

TF: Technical functions

SU: Sectors of use PROC: Process categories AC: Article categories

Revision No: 101 - Replaces version: 101