

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 1 of 11

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:	Andreas Goertz	Telephone: + 49 2822 68561 37
e-mail:	andreas.goertz@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	QM - Regulatory Affairs	

1.4. Emergency telephone number:

+49 2822 68561 99

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
 Aquatic Acute 1; H400

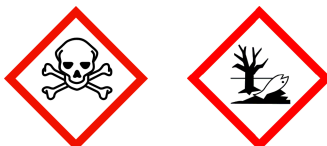
Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Danger

Pictograms:



Hazard statements

H301+H311 Toxic if swallowed or in contact with skin.
 H400 Very toxic to aquatic life.

Precautionary statements

P264 Wash 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.
 P330 Rinse mouth.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 2 of 11

P302+P352	IF ON SKIN: Wash with plenty of water.
P312	Call a POISON CENTER/doctor if you feel unwell.
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 .

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C ₉ H ₁₆ O ₂
Molecular weight:	156,22

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)			100 %
	204-642-4			
	Acute Tox. 3, Acute Tox. 3, Aquatic Acute 1; H311 H301 H400			

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 water. Induce vomiting when the affected person is not unconscious. Call a physician immediately.

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.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 3 of 11

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.

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. Do not breathe gas/fumes/vapour/spray. Avoid contact with skin, eyes and clothes. Use personal protection equipment.

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

For cleaning up

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.

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. 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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 4 of 11

adequate ventilation as well as local exhaust 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	Exposure route	Effect	Value
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)		
Worker DNEL, long-term	inhalation	systemic	15 mg/m ³
Worker DNEL, long-term	dermal	systemic	4,3 mg/kg bw/day
Consumer DNEL, long-term	inhalation	systemic	3,7 mg/m ³
Consumer DNEL, long-term	dermal	systemic	2,1 mg/kg bw/day
Consumer DNEL, long-term	oral	systemic	2,1 mg/kg bw/day

PNEC values

CAS No	Name of agent	
Environmental compartment	Value	
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	
Marine water	0,000012 mg/l	
Freshwater sediment	0,00446 mg/kg	
Marine sediment	0,000446 mg/kg	
Secondary poisoning	47,56 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/face protection.

Hand protection

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)

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 5 of 11

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 point:	<-20 °C
Boiling point or initial boiling point and boiling range:	187 °C
Flammability	
Solid/liquid:	not applicable
Gas:	not applicable
Lower explosion limits:	not determined
Upper explosion limits:	not determined
Flash point:	63 °C
Auto-ignition temperature:	268 °C
Decomposition temperature:	not determined
pH-Value:	not determined
Viscosity / kinematic: (at 20 °C)	1,22 mm ² /s
Water solubility: (at 20 °C)	0,41 g/L
Solubility in other solvents	
not determined	
Partition coefficient n-octanol/water:	3,2
Vapour pressure: (at 20 °C)	2,69 hPa
Density (at 20 °C):	0,89 g/cm ³
Relative vapour density: (at 20 °C)	5,39

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

The product is not: Explosive. not explosive according to EU A.14

Oxidizing properties

The product is not: oxidising.

Other safety characteristics

Evaporation rate:	not determined
Solvent content:	0%
Solid content:	0%
Viscosity / dynamic: (at 20 °C)	1,09 mPa·s

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.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 6 of 11

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 HEXANOATE (CAPROATE)				
	oral	LD50 218 mg/kg	Rat	REACH Dossier	OECD 401
	dermal	LD50 820 mg/kg	Rabbit	REACH Dossier	OECD 402

Irritation and corrosivity

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

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

12.1. Toxicity

Very toxic to aquatic life.

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 7 of 11

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 OECD 203
	Acute algae toxicity	ErC50 mg/l	>4,6	72 h	Desmodesmus subspicatus	REACH Registration OECD 201
	Acute crustacea toxicity	EC50	2,0 mg/l	48 h	Daphnia magna (Big water flea)	REACH Registration EU Method C.2
	Algae toxicity	NOEC mg/l	0,158	72 d	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.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 8 of 11

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

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 - 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
<u>14.2. UN proper shipping name:</u>	TOXIC LIQUID, ORGANIC, N.O.S.
<u>14.3. Transport hazard class(es):</u>	6.1
<u>14.4. Packing group:</u>	III
Hazard label:	6.1



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 transport)
E1

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	UN 2810
<u>14.2. UN proper shipping name:</u>	TOXIC LIQUID, ORGANIC, N.O.S.
<u>14.3. Transport hazard class(es):</u>	6.1
<u>14.4. Packing group:</u>	III
Hazard label:	6.1



Classification code:	T1
Special Provisions:	274 614 802
Limited quantity:	5 L
Excepted quantity:	E1

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 9 of 11

Other applicable information (inland waterways transport)

E1

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



Special Provisions:	223, 274
Limited quantity:	5 L
Excepted quantity:	E1
EmS:	F-A, S-A

Air transport (ICAO-TI/IATA-DGR)

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



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

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



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

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 3

2010/75/EU (VOC): 100 % (890 g/l)

2004/42/EC (VOC): 100 % (890 g/l)

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 10 of 11

Information according to 2012/18/EU (SEVESO III):

E1 Hazardous to the Aquatic Environment

Additional information

To follow: 850/2004/EC, 79/117/EEC, 689/2008/EC

National regulatory information

Employment restrictions:

Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

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): 2,4,6,7,8,9,11,12,16.

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

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

DNEL: 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

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 01.06.2022

Product code: 203210

Page 11 of 11

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).

Relevant H and EUH statements (number and full text)

H301	Toxic if swallowed.
H301+H311	Toxic if swallowed or in contact with skin.
H311	Toxic in contact with skin.
H400	Very toxic to aquatic life.

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
1	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