

according to Regulation (EC) No 1907/2006

NATURAL ALLYL HEXANOATE (CAPROATE)

Revision date: 21.06.2024 Product code: 203210 Page 1 of 12

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 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: Danger

Pictograms:





Hazard statements

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

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

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.

Print date: 09.10.2024



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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	Chemical name					
	EC No Index No REACH No						
	Classification (Regulation (EC) No 1272/2008)						
123-68-2	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

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CAS No	EC No	EC No Chemical name						
	Specific Conc.	Specific Conc. Limits, M-factors and ATE						
123-68-2	204-642-4	204-642-4 NATURAL ALLYL HEXANOATE (CAPROATE)						
	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		Exposure route	Effect	Value				
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)							
Worker DNEL,	long-term	inhalation	systemic	15 mg/m³				
Worker DNEL,	long-term	dermal	systemic	4,3 mg/kg bw/day				
Consumer DNEL, long-term		inhalation	systemic	3,7 mg/m³				
Consumer DN	EL, long-term	dermal	systemic	2,1 mg/kg bw/day				
Consumer DN	EL, long-term	oral	systemic	2,1 mg/kg bw/day				

PNEC values

CAS No	Name of agent					
Environment	Environmental compartment					
123-68-2 NATURAL ALLYL HEXANOATE (CAPROATE)						
Freshwater	0,00012 mg/l					
Marine water	0,000012 mg/l					
Freshwater s	0,00446 mg/kg					
Marine sedim	0,000446 mg/kg					
Micro-organis	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 point: <-20 °C
Boiling point or initial boiling point and 187 °C

boiling range:

Flammability: not determined Lower explosion limits: not determined Upper explosion limits: not determined 63 °C Flash point: 268 °C Auto-ignition temperature: Decomposition temperature: not determined not determined pH-Value: Viscosity / kinematic: 1.22 mm²/s

(at 20 °C)

Water solubility: 0,41 g/l

(at 20 °C)

Solubility in other solvents

not determined

Partition coefficient n-octanol/water:

Vapour pressure:

3,2

2,69 hPa

(at 20 °C)

Density (at 20 °C):

Relative vapour density:

0,89 g/cm³

5,39

(at 20 °C)

Particle characteristics: not applicable

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: 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	Chemical name									
	Exposure route	Exposure route Dose Species Source Method									
123-68-2	NATURAL ALLYL HEXA	NATURAL ALLYL HEXANOATE (CAPROATE)									
	oral	LD50 218 mg/kg		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	Chemical name								
	Aquatic toxicity	Dose		[h] [d]	Species	Source	Method			
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)			DATE)						
	Acute fish toxicity	LC50 0,117 mg/l		96 h	Danio rerio (zebrafish)	REACH Registration	OEDC 203			
	Acute algae toxicity	ErC50 >4,6 mg/l		I . — · ·	Desmodesmus subspicatus	REACH Registration	OECD 201			
	Acute crustacea toxicity	EC50 2,0 mg/l	EC50 2,0 mg/l	2,0 mg/l 48 h Daphnia magna (Big water flea)		2,0 mg/l			na (Big REACH OECD 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 RE							
	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
	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

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)

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):6.114.4. Packing group:IIIHazard 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)

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:
Hazard label:
6.1



Classification code:



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Special Provisions: 274 614 802
Limited quantity: 5 L

Excepted quantity: E1

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):6.114.4. Packing group:IIIHazard 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):6.114.4. Packing group:IIIHazard label:6.1



Special Provisions:

A3 A4 A137

Limited quantity Passenger:

Passenger LQ:

Y642

Excepted quantity:

E1

IATA-packing instructions - Passenger:655IATA-max. quantity - Passenger:60 LIATA-packing instructions - Cargo:663IATA-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



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Directive 2010/75/EU on industrial

emissions:

100 % (890 g/l)

Directive 2004/42/EC on VOC in

100 % (890 g/l)

paints and varnishes:

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, 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.

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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

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

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.

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



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H311 Toxic in contact with skin. H400 Very toxic to aquatic life.

H410 Very 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
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