

according to 29 CFR 1910.1200(g)

NATURAL ALLYL HEXANOATE (CAPROATE)

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1. Identification

Product identifier

NATURAL ALLYL HEXANOATE (CAPROATE)

Substance name: NATURAL ALLYL HEXANOATE (CAPROATE)

CAS No: 123-68-2

Recommended use of the chemical and restrictions on use

Use of the substance/mixture

For Flavour use for food and feed only

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

Emergency phone number: +49 2822 68561 99

2. Hazard(s) identification

Classification of the chemical

29 CFR Part 1910.1200

Acute toxicity: Acute Tox. 3 (dermal)
Acute toxicity: Acute Tox. 3 (oral)

Hazardous to the aquatic environment: Aquatic Acute 1

Label elements

29 CFR Part 1910.1200

Signal word: Danger

Pictograms:



Hazard statements

Combustible liquid

Toxic if swallowed or in contact with skin

Precautionary statements

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

Wash hands thoroughly after handling.

Do not eat, drink or smoke when using this product.

Wear protective gloves/protective clothing/eye protection/face protection.

If swallowed: Immediately call a poison center/doctor.

Rinse mouth.

If on skin: Wash with plenty of water.

Call a poison center/doctor if you feel unwell.

Take off immediately all contaminated clothing and wash it before reuse.

In case of fire: Use Water spray jet / alcohol resistant foam / Dry extinguishing powder / Carbon dioxide (CO2)

to extinguish.



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Store in a well-ventilated place.

Store locked up.

Dispose of contents/container to Organic waste.

Hazards not otherwise classified

No information available.

3. Composition/information on ingredients

Substances

Sum formula: C9 H16 O2 Molecular weight: 156,22

Hazardous components

CAS No	Components	Quantity
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	100 %

4. First-aid measures

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.

Most important symptoms and effects, both acute and delayed

No information available.

Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

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

Specific hazards arising from the chemical

Non-flammable. Vapors may form explosive mixtures with air.

Special protective equipment and precautions for fire-fighters

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

Additional information

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



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6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

General advice

Provide adequate ventilation. Do not breathe gas/fume/vapor/spray. Avoid contact with skin, eyes and clothes. Use personal protection equipment.

Environmental precautions

Do not allow to enter into surface water or drains.

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.

Reference to other sections

Safe handling: see section 7

Personal protection equipment (PPE): see section 8

Disposal: see section 13

7. Handling and storage

Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fume/vapor/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.

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.

8. Exposure controls/personal protection

Control parameters

Exposure controls





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Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fume/vapor/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)

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

9. Physical and chemical properties

Information on basic physical and chemical properties

Physical state: Liquid

Color: Colourless to pale yellow

Odor: pineapple

Changes in the physical state

Melting point/freezing point: <-20 °C
Boiling point or initial boiling point and 187 °C

boiling range:

Flash point: 63 °C

Flammability

Solid/liquid: not applicable
Gas: not applicable

Explosive properties

The product is not: Explosive. not hazard of explosion according to EU A.14

Lower explosion limits:

Upper explosion limits:

not determined

Auto-ignition temperature:

not determined

Decomposition temperature:

not determined

pH-Value:

not determined

viscosity / dynamic:

1,09 mPa·s

(at 20 °C)

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: 3,2



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Vapor pressure: 2,69 hPa

(at 20 °C)

Density (at 20 °C): 0,89 g/cm³
Relative vapour density: 5,39

(at 20 °C)

Other information

Information with regard to physical hazard classes

Oxidizing properties

The product is not: oxidising.

Other safety characteristics

Solvent content: 0%
Solid content: 0%
Evaporation rate: not determined

10. Stability and reactivity

Reactivity

No hazardous reaction when handled and stored according to provisions.

Chemical stability

The product is stable under storage at normal ambient temperatures.

Possibility of hazardous reactions

No known hazardous reactions.

Conditions to avoid

none/none

Incompatible materials

No information available.

Hazardous decomposition products

No known hazardous decomposition products.

11. Toxicological information

Information on toxicological effects

Acute toxicity

Toxic if swallowed

Toxic in contact with skin

CAS No	Components						
	Exposure route	Dose		Species	Source	Method	
123-68-2	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

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

Sensitizing 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.



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Specific target organ toxicity (STOT) - single exposure

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

Specific target organ toxicity (STOT) - repeated exposure

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

Carcinogenicity (OSHA): Not listed.
Carcinogenicity (IARC): Not listed.
Carcinogenicity (NTP): Not listed.

Aspiration hazard

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

12. Ecological information

Ecotoxicity

Very toxic to aquatic life.

CAS No	Components						
	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	72 h	Desmodesmus subspicatus	REACH Registration	OECD 201
	Acute crustacea toxicity	EC50	2,0 mg/l		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

Persistence and degradability

The product has not been tested.

Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

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

BCF

CAS No	Components	BCF	Species	Source
	NATURAL ALLYL HEXANOATE (CAPROATE)	102,3	Fish	REACH Registration

Mobility in soil

The product has not been tested.

Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

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.

13. Disposal considerations

Waste treatment methods



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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.

Contaminated packaging

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

14. Transport information

U.S. DOT 49 CFR 172.101

UN number or ID number: UN 2810

Proper shipping name: TOXIC LIQUIDS, ORGANIC, N.O.S.

Transport hazard class(es):

Packing group:
Hazard label:

6.1

6.1

6.1



Marine transport (IMDG)

UN number or ID number: UN 2810

<u>UN proper shipping name:</u> TOXIC LIQUID, ORGANIC, N.O.S.

Transport hazard class(es):6.1Packing 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)

UN number or ID number: UN 2810

UN proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S.

Transport hazard class(es):6.1Packing group:IIIHazard label:6.1



Special Provisions:
A3 A4 A137
Limited quantity Passenger:
2 L
Passenger LQ:
Y642

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

Environmental hazards



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ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: ALLYL HEXANOATE

Special precautions for user

Warning: Acute Toxicity.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

not applicable

15. Regulatory information

U.S. Regulations

National regulatory information

SARA Section 311/312 Hazards:

NATURAL ALLYL HEXANOATE (CAPROATE) (123-68-2): Immediate (acute) health hazard

State Regulations

Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65, State of California)

This product can not expose you to chemicals known to the State of California to cause cancer, birth defects or other reproductive harm.

16. Other information

Changes

Revision date: 01.06.2022 Revision No: 101

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



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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).

Other data

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.