

Safety Data Sheet

according to UN GHS (ST/SG/AC.10/11/Rev.10)

NATURAL ALLYL HEXANOATE (CAPROATE) 25%

Revision date: 25.08.2022

Product code: 203200WW

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

1.1. Product identifier

NATURAL ALLYL HEXANOATE (CAPROATE) 25%

CAS No: 123-68-2

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 number:

+49 2822 68561 99

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

UN GHS (ST/SG/AC.10/11/Rev.10)

Flammable liquid: Flam. Liq. 2
 Acute toxicity: Acute Tox. 4 (oral)
 Acute toxicity: Acute Tox. 5 (dermal)
 Serious eye damage/eye irritation: Eye Irrit. 2
 Hazardous to the aquatic environment: Aquatic Acute 1
 Hazardous to the aquatic environment: Aquatic Chronic 3

2.2. Label elements

UN GHS (ST/SG/AC.10/11/Rev.10)

Hazard components for labelling

NATURAL ALLYL HEXANOATE (CAPROATE)

Signal word: Danger

Pictograms:



Hazard statements

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H313	May be harmful in contact with skin.
H319	Causes serious eye irritation.
H400	Very toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary statements

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
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P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharges.
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+P317	IF SWALLOWED: Get medical help.
P330	Rinse mouth.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
P317	Get medical help.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337+P317	If eye irritation persists: Get medical help.
P391	Collect spillage.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container to organic waste.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Relevant ingredients

CAS No	Chemical name	Quantity
	Classification (UN GHS (ST/SG/AC.10/11/Rev.10))	
64-17-5	ethanol, ethyl alcohol	65 - < 70 %
	Flam. Liq. 2, Eye Irrit. 2; H225 H319	
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	25 - < 30 %
	Acute Tox. 3, Acute Tox. 3, Aquatic Acute 1, Aquatic Chronic 3; H311 H301 H400 H412	
105-54-4	NATURAL ETHYL BUTYRATE	10 - < 15 %
	Flam. Liq. 3, Eye Irrit. 2; H226 H319	

SECTION 4: First aid measures

4.1. Description of first aid measures

After inhalation

Provide fresh air.

After contact with skin

Wash with plenty of water. Take off contaminated clothing and wash it before reuse.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately.

After ingestion

Observe risk of aspiration if vomiting occurs. Rinse mouth immediately and drink 1 glass of water. Medical treatment necessary.

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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

Carbon dioxide (CO₂), Foam, Extinguishing powder.

Unsuitable extinguishing media

Water.

5.2. Special hazards arising from the substance or mixture

Highly flammable. Vapours can form explosive mixtures with air.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

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

Remove all sources of ignition. 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 uncontrolled discharge of product into the environment. Explosion risk.

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

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges. Vapours can form explosive mixtures with air.

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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 in a cool, well-ventilated place. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints on joint storage

Do not store together with: Oxidizing agent. Pyrophoric or self-heating substances.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls



Individual protection measures, such as personal protective equipment

Eye/face protection

Suitable eye protection: goggles.

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.

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Thermal hazards

Flame-retardant protective clothing. Wear anti-static footwear and clothing

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:		>78 °C
Flammability:		not applicable
Lower explosion limits:		not applicable
Upper explosion limits:		>1,5 vol. %
Flash point:		<27,7 vol. %
Auto-ignition temperature:		>13 °C
		~368 °C

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Decomposition temperature:	not determined
pH-Value:	not determined
Water solubility:	The study does not need to be conducted because the substance is known to be insoluble in water.
Solubility in other solvents	
not determined	
Partition coefficient n-octanol/water:	not determined
Vapour pressure:	<58 hPa
(at 20 °C)	
Vapour pressure:	<293 hPa
(at 50 °C)	
Density (at 20 °C):	0,82 g/cm ³
Relative vapour density:	not determined

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: 65,00 %

Solid content: 0%

SECTION 10: Stability and reactivity

10.1. Reactivity

Highly flammable.

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

Keep away from sources of heat (e.g. hot surfaces), sparks and open flames. Vapours can form explosive mixtures with air.

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 toxicological effects

Acute toxicity

Harmful if swallowed.

May be harmful in contact with skin.

ATEmix calculated

ATE (oral) 872,0 mg/kg; ATE (dermal) 3280 mg/kg; ATE (inhalation vapour) > 50 mg/l; ATE (inhalation dust/mist) > 12,5 mg/l

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
64-17-5	ethanol, ethyl alcohol				
	oral	LD50 mg/kg	10470	Rat	REACH Dossier OECD 401
	dermal	LD50 mg/kg	17100	Rabbit	REACH Dossier
	inhalation (4 h) vapour	LC50	121 mg/l	Rat	REACH Dossier OECD 403
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
105-54-4	NATURAL ETHYL BUTYRATE				
	oral	LD50 mg/kg	>2000	Rat	REACH Registration OECD 423
	dermal	LD50 mg/kg	>2000	Rat	REACH Registration OECD 402
	inhalation (1 h) vapour	LC50	>7380	Rat	REACH Registration

Irritation and corrosivity

Serious eye damage/eye irritation: Causes serious eye irritation.

Skin corrosion/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.

Further information

The mixture is classified as hazardous according to regulation (EC) No 1272/2008 [CLP].

SECTION 12: Ecological information

12.1. Toxicity

Very toxic to aquatic life.

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CAS No	Chemical name					
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method
64-17-5	ethanol, ethyl alcohol					
	Acute fish toxicity	LC50 mg/l	14200	96 h	Pimephales promelas (fathead minnow)	REACH Dossier US EPA method E03-05
	Acute algae toxicity	ErC50	275 mg/l	72 h	Chlorella vulgaris	REACH Dossier OECD 201
	Acute crustacea toxicity	EC50 mg/l	5012	48 h	Ceriodaphnia spec	REACH Dossier ASTM E729-80
	Fish toxicity	NOEC	250 mg/l	5 d	Danio rerio (zebrafish)	REACH Dossier OECD 212
	Crustacea toxicity	NOEC	9,6 mg/l	9 d	Daphnia magna	REACH Dossier
	Acute bacteria toxicity	EC50 mg/l ()	>1000	3 h	Activated sludge	REACH Dossier OECD 209
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 OECD TG 202
	Algae toxicity	NOEC mg/l	0,158	72 d	Desmodesmus subspicatus	REACH Registration OECD 201
105-54-4	NATURAL ETHYL BUTYRATE					
	Acute fish toxicity	LC50 mg/l	>100	96 h	Danio rerio (zebrafish)	REACH Registration OECD 203
	Acute algae toxicity	ErC50	100 mg/l	72 h	Desmodesmus subspicatus	REACH Registration OECD 201
	Acute crustacea toxicity	EC50 mg/l	116,6	48 h	Daphnia magna (Big water flea)	REACH Registration OECD 202
	Fish toxicity	NOEC mg/l	1483	28 d	fish species (undefined)	REACH Registration
	Crustacea toxicity	NOEC mg/l	28833	21 d	Daphnia magna (Big water flea)	REACH Registration

12.2. Persistence and degradability

The product has not been tested.

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CAS No	Chemical name			
	Method	Value	d	Source
	Evaluation			
64-17-5	ethanol, ethyl alcohol			
	OECD 301B	95%	28	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301B	84%	20	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
	OECD 301B	74%	5	REACH Dossier
	Readily biodegradable (according to OECD criteria).			
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).			
105-54-4	NATURAL ETHYL BUTYRATE			
	OECD 301D	25%	7	REACH Registration
	Moderately/partially biodegradable.			
	OECD 301D	53,18%	14	REACH Registration
	Moderately/partially biodegradable.			
	OECD 301D	55,9%	28	REACH Registration
	Moderately/partially biodegradable.			

12.3. Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
64-17-5	ethanol, ethyl alcohol	-0,3
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	3,191
105-54-4	NATURAL ETHYL BUTYRATE	2,43

BCF

CAS No	Chemical name	BCF	Species	Source
64-17-5	ethanol, ethyl alcohol	1-4,5	Cyprinus carpio (Common Carp)	REACH Registration
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	102,3	Fish	REACH Registration
105-54-4	NATURAL ETHYL BUTYRATE	8	-	REACH Registration

12.4. Mobility in soil

The product has not been tested.

12.6. Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

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.

Contaminated packaging

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information

Marine transport (IMDG)

14.1. UN number or ID number:	UN 3272
14.2. UN proper shipping name:	ESTERS, N.O.S.
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3



Special Provisions:	274
Limited quantity:	1 L
Excepted quantity:	E2
EmS:	F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:	UN 3272
14.2. UN proper shipping name:	ESTERS, N.O.S.
14.3. Transport hazard class(es):	3
14.4. Packing group:	II
Hazard label:	3



Special Provisions:	A3
Limited quantity Passenger:	1 L
Passenger LQ:	Y341
Excepted quantity:	E2
IATA-packing instructions - Passenger:	353
IATA-max. quantity - Passenger:	5 L
IATA-packing instructions - Cargo:	364
IATA-max. quantity - Cargo:	60 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

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not applicable

SECTION 15: Regulatory information**National regulatory information**

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC).

SECTION 16: Other information**Changes**

This data sheet contains changes from the previous version in section(s): 14,15.

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
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).

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of

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product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

(The data for the relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)