

Safety Data Sheet

according to 29 CFR 1910.1200(g)

NATURAL ALLYL HEXANOATE (CAPROATE) 25%

Revision date: 08/25/2022

Product code: 203200US

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1. Identification

Product identifier

NATURAL ALLYL HEXANOATE (CAPROATE) 25%

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:	Safety Team	Telephone: + 49 2822 68561 0
E-mail:	safety-documentation@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	Safety Management	

Emergency phone number: +49 2822 68561 99

2. Hazard(s) identification

Classification of the chemical

29 CFR Part 1910.1200

Flammable liquids: Flam. Liq. 2
 Acute toxicity: Acute Tox. 4 (oral)
 Serious eye damage/eye irritation: Eye Irrit. 2A

Label elements

29 CFR Part 1910.1200

Signal word: Danger

Pictograms:



Hazard statements

Highly flammable liquid and vapor
 Harmful if swallowed
 Causes serious eye irritation

Precautionary statements

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
 Keep container tightly closed.
 Ground/bond container and receiving equipment.
 Use explosion-proof electrical/ventilating/lighting equipment.
 Use only non-sparking tools.
 Take precautionary measures against static discharge.
 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: Call a poison center/doctor if you feel unwell.
 Rinse mouth.

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If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.
 Continue rinsing.
 If eye irritation persists: Get medical advice/attention.
 Store in a well-ventilated place. Keep cool.
 Dispose of contents/container to Organic waste.

Hazards not otherwise classified

No information available.

3. Composition/information on ingredients

Mixtures

Relevant ingredients

CAS No	Components	Quantity
64-17-5	ethanol, ethyl alcohol	60 - 67,5 %
123-68-2	NATURAL ALLYL HEXANOATE (CAPROATE)	25 - 27,5 %
105-54-4	NATURAL ETHYL BUTYRATE	7,5 - 12,5 %

4. First-aid measures

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.

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

Carbon dioxide (CO2), Foam, Extinguishing powder.

Unsuitable extinguishing media

Water.

Specific hazards arising from the chemical

Highly flammable. Vapors may form explosive mixtures with air.

Special protective equipment and precautions for fire-fighters

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/vapors/mists with water spray jet. Collect contaminated fire extinguishing water separately. Do not allow entering drains or

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surface water.

6. Accidental release measures**Personal precautions, protective equipment and emergency procedures****General advice**

Remove all sources of ignition. Do not breathe gas/fume/vapor/spray. Avoid contact with skin, eyes and clothes. Use personal protection equipment.

Environmental precautions

Do not allow uncontrolled discharge of product into the environment. Explosion risk.

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

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

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 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.

8. Exposure controls/personal protection**Control parameters**

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Exposure limits

CAS No	Substance	ppm	mg/m ³	Category	Origin
64-17-5	Ethanol	1000	1880	STEL (15 min)	ACGIH-2024
64-17-5	Ethyl alcohol (Ethanol)	1000	1900	TWA (8 h)	PEL
64-17-5	Ethyl alcohol	1000	1900	TWA (8 h)	REL

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

9. Physical and chemical properties

Information on basic physical and chemical properties

Physical state:	Liquid
Color:	Colourless to pale yellow
Odor:	pineapple
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
Decomposition temperature:	~368 °C
pH-Value:	not determined
Water solubility:	not determined
Solubility in other solvents:	The study does not need to be conducted because the substance is known to be insoluble in water.
Partition coefficient n-octanol/water:	not determined

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Vapor pressure: (at 20 °C)	<58 hPa
Vapor pressure: (at 50 °C)	<293 hPa
Density (at 20 °C):	0,82 g/cm ³
Relative vapour density:	not determined

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%

10. Stability and reactivity**Reactivity**

Highly flammable.

Chemical stability

The product is stable under storage at normal ambient temperatures.

Possibility of hazardous reactions

No known hazardous reactions.

Conditions to avoid

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

Incompatible materials

No information available.

Hazardous decomposition products

No known hazardous decomposition products.

11. Toxicological information**Information on toxicological effects****Acute toxicity**

Harmful if swallowed

ATEmix calculated

ATE (oral) 842,6 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

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CAS No	Components				
	Exposure route	Dose	Species	Source	Method
64-17-5	ethanol, ethyl alcohol				
	oral	LD50 10470 mg/kg	Rat	REACH Dossier	OECD 401
	dermal	LD50 17100 mg/kg	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 218 mg/kg	Rat	REACH Dossier	OECD 401
	dermal	LD50 820 mg/kg	Rabbit	REACH Dossier	OECD 402
105-54-4	NATURAL ETHYL BUTYRATE				
	oral	LD50 >2000 mg/kg	Rat	REACH Registration	OECD 423
	dermal	LD50 >2000 mg/kg	Rat	REACH Registration	OECD 402
	inhalation (1 h) vapour	LC50 >7380 mg/l	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.

Sensitizing 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.

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):

No ingredient of this mixture is listed.

Carcinogenicity (IARC):

Ethanol in alcoholic beverages (CAS 64-17-5) is listed in group 1.

Carcinogenicity (NTP):

No ingredient of this mixture is listed.

Aspiration hazard

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

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].

12. Ecological information

Ecotoxicity

Very toxic to aquatic life.

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CAS No	Components					
	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

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
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	Components	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

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Mobility in soil

The product has not been tested.

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.

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

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.

14. Transport information

U.S. DOT 49 CFR 172.101

<u>UN number or ID number:</u>	UN 3272
<u>Proper shipping name:</u>	ESTERS, N.O.S.
<u>Transport hazard class(es):</u>	3
<u>Packing group:</u>	II
Hazard label:	3



Marine transport (IMDG)

<u>UN number or ID number:</u>	UN 3272
<u>UN proper shipping name:</u>	ESTERS, N.O.S.
<u>Transport hazard class(es):</u>	3
<u>Packing group:</u>	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)

<u>UN number or ID number:</u>	UN 3272
<u>UN proper shipping name:</u>	ESTERS, N.O.S.
<u>Transport hazard class(es):</u>	3
<u>Packing group:</u>	II
Hazard label:	3

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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

Environmental hazards

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:

ethanol, ethyl alcohol (64-17-5): Fire hazard, Immediate (acute) health hazard

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

NATURAL ETHYL BUTYRATE (105-54-4): Fire hazard, 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: 08/25/2022

Revision No: 103

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

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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).

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.

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