

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ALPHA-IONONE

Revision date: 07.06.2024

Product code: 259420

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

1.1. Product identifier

NATURAL ALPHA-IONONE

Substance name:	NATURAL ALPHA-IONONE
CAS No:	127-41-3
EC No:	204-841-6
UFI:	QDF5-1RXT-700T-4MYU

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture

Manufacturing of: - Air care products - Perfumes, fragrances - Pharmaceuticals - Cosmetics, personal care products - Flavouring Substances - Other

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 143
E-mail:	andreas.goertz@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	QM - Regulatory Affairs - Safety Management	

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

Aquatic Chronic 3; H412

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

P273	Avoid release to the environment.
P501	Dispose of contents/container to organic waste.

2.3. Other hazards

Contains no substances of very high concern (SVHC) which are included in the Candidate List according to Article 59 of REACH. Contains no substances of very high concern (SVHC) which are subject to authorisation according to Annex XIV of REACH.

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Sum formula:	C13 H20 O
Molecular weight:	192,30

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Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
127-41-3	NATURAL ALPHA-IONONE			95,0 - 99,0%
	204-841-6			
14901-07-6	NATURAL BETA-IONONE			1,0 - 5,0%
	238-969-9			
	Aquatic Chronic 2; H411			

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		
127-41-3	204-841-6	NATURAL ALPHA-IONONE	95,0 - 99,0%
	dermal: LD50 = >5000 mg/kg; oral: LD50 = 4590 mg/kg		
14901-07-6	238-969-9	NATURAL BETA-IONONE	1,0 - 5,0%
	inhalation: LC50 = 538,49 mg/l (vapours); dermal: LD50 = 5331 mg/kg; oral: LD50 = 4590 mg/kg		

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

Rinse immediately carefully and thoroughly with eye-bath or water.

After ingestion

Rinse mouth immediately and drink 1 glass of water.

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.

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. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

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SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****General advice**

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**

No special measures are necessary.

Advice on protection against fire and explosion

No special fire protection measures are necessary.

Advice on general occupational hygiene

Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink, smoke, sniff. Take off contaminated clothing. Wash hands before breaks and after work. 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.

Hints on joint storage

No special measures are necessary.

7.3. Specific end use(s)

Manufacturing of: - Air care products - Perfumes, fragrances - Pharmaceuticals - Cosmetics, personal care products - Flavouring Substances - Other

SECTION 8: Exposure controls/personal protection**8.1. Control parameters**

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DNEL/DMEL values

CAS No	Name of agent		
DNEL type	Exposure route	Effect	Value
127-41-3	NATURAL ALPHA-IONONE		
Worker DNEL, long-term	inhalation	systemic	0,987 mg/m ³
Worker DNEL, long-term	dermal	systemic	0,28 mg/kg bw/day
Consumer DNEL, long-term	inhalation	systemic	0,174 mg/m ³
Consumer DNEL, long-term	dermal	systemic	0,1 mg/kg bw/day
Consumer DNEL, long-term	oral	systemic	0,1 mg/kg bw/day
14901-07-6	NATURAL BETA-IONONE		
Worker DNEL, long-term	inhalation	systemic	2,498 mg/m ³
Worker DNEL, long-term	dermal	systemic	2,191 mg/kg bw/day
Consumer DNEL, long-term	inhalation	systemic	0,621 mg/m ³
Consumer DNEL, long-term	dermal	systemic	0,54 mg/kg bw/day
Consumer DNEL, long-term	oral	systemic	4,383 mg/kg bw/day

PNEC values

CAS No	Name of agent	
Environmental compartment	Value	
127-41-3	NATURAL ALPHA-IONONE	
Freshwater	0,0034 mg/l	
Marine water	0,0003 mg/l	
Freshwater sediment	0,984 mg/kg	
Marine sediment	0,0944 mg/kg	
Micro-organisms in sewage treatment plants (STP)	13,1 mg/l	
Soil	0,195 mg/kg	
14901-07-6	NATURAL BETA-IONONE	
Freshwater	0,001 mg/l	
Freshwater (intermittent releases)	0,015 mg/l	
Marine water	0 mg/l	
Freshwater sediment	22,451 mg/l	
Marine sediment	22,451 mg/l	
Micro-organisms in sewage treatment plants (STP)	0,043 mg/l	
Soil	10,466 mg/kg	

8.2. Exposure controls

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear eye protection/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

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supplier of these gloves.

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:		
		Test method
Melting point/freezing point:	-16 °C	
Boiling point or initial boiling point and boiling range:	237 °C	
Flammability:	not determined	
Lower explosion limits:	not determined	
Upper explosion limits:	not determined	
Flash point:	87 °C	
Auto-ignition temperature:	not determined	
Decomposition temperature:	not determined	
pH-Value (at 29 °C):	4,55	OECD 122
Viscosity / kinematic: (at 20 °C)	41,15 mm ² /s	
Water solubility: (at 25 °C)	0,059 g/L	
Solubility in other solvents	not determined	
Partition coefficient n-octanol/water:	3,896	
Vapour pressure: (at 20 °C)	0,0013 hPa	
Density (at 20 °C):	0,93 g/cm ³	
Relative vapour density: (at 20 °C)	7	
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: (at 20 °C)	36,45 mPa·s

SECTION 10: Stability and reactivity

10.1. Reactivity

No hazardous reaction when handled and stored according to provisions.

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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

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

ATEmix calculated

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

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
127-41-3	NATURAL ALPHA-IONONE				
	oral	LD50 mg/kg	4590	Rat	REACH Dossier
	dermal	LD50 mg/kg	>5000	Rabbit	REACH Dossier
14901-07-6	NATURAL BETA-IONONE				
	oral	LD50 mg/kg	4590	Rat	REACH Dossier
	dermal	LD50 mg/kg	5331	Mouse	REACH Dossier
	inhalation (4 h) vapour	LC50 mg/l	538,49	Rat	REACH Dossier

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.

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11.2. Information on other hazards

Endocrine disrupting properties

No information available.

SECTION 12: Ecological information

12.1. Toxicity

Harmful to aquatic life with long lasting effects.

Harmful to aquatic life with long lasting effects.

CAS No	Chemical name						
	Aquatic toxicity	Dose	[h] [d]	Species	Source	Method	
127-41-3	NATURAL ALPHA-IONONE						
	Acute fish toxicity	LC50 6,8 mg/l	96 h	Leuciscus idus (golden orfe)	REACH Dossier		
	Acute algae toxicity	ErC50 mg/l 22,2	72 h	Desmodesmus subspicatus	REACH Dossier		
	Acute crustacea toxicity	EC50 mg/l 2,65	48 h	Daphnia magna (Big water flea)	REACH Dossier		
	Fish toxicity	NOEC mg/l 0,173	28 d	fish species (undefined)	REACH Dossier		
	Crustacea toxicity	NOEC mg/l 0,17	21 d	freshwater invertebrates	REACH Dossier		
14901-07-6	NATURAL BETA-IONONE						
	Acute fish toxicity	LC50 mg/l 2,571	96 h	Oryzias latipes (Ricefish)	REACH Dossier		
	Acute algae toxicity	ErC50 mg/l 3,223	72 h	Pseudokirchneriella subcapitata	REACH Dossier		
	Acute crustacea toxicity	EC50 mg/l 1,641	48 h	Daphnia magna (Big water flea)	REACH Dossier		

12.2. Persistence and degradability

The product has not been tested.

CAS No	Chemical name				
	Method	Value	d	Source	
	Evaluation				
127-41-3	NATURAL ALPHA-IONONE				
	OECD 301B	75,4%	28	REACH Dossier	
	inherently biodegradable				
14901-07-6	NATURAL BETA-IONONE				
		50%	38	REACH Dossier	
	Not 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
127-41-3	NATURAL ALPHA-IONONE	3,896
14901-07-6	NATURAL BETA-IONONE	3,84

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BCF

CAS No	Chemical name	BCF	Species	Source
127-41-3	NATURAL ALPHA-IONONE	161	Fish	REACH Dossier
14901-07-6	NATURAL BETA-IONONE	159		REACH Dossier

12.4. Mobility in soil

The product has not been tested.

12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

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.

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

Non-contaminated packages may be recycled. 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>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

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<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

<u>14.1. UN number or ID number:</u>	No dangerous good in sense of this transport regulation.
<u>14.2. UN proper shipping name:</u>	No dangerous good in sense of this transport regulation.
<u>14.3. Transport hazard class(es):</u>	No dangerous good in sense of this transport regulation.
<u>14.4. Packing group:</u>	No dangerous good in sense of this transport regulation.

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



Danger releasing substance: NATURAL ALPHA-IONONE

14.6. Special precautions for user

No information available.

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

Directive 2004/42/EC on VOC in paints and varnishes: 97,5 % (906,75 g/l)

Information according to Directive 2012/18/EU (SEVESO III): Not subject to 2012/18/EU (SEVESO III)

National regulatory information

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

Water hazard class (D): 2 - obviously hazardous to water

15.2. Chemical safety assessment

Chemical safety assessments for substances in this mixture were not carried out.

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 1,7,11,12.

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Abbreviations and acronyms

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>
 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
 For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety
 assessment, chapter R.20 (Table of terms and abbreviations).

Classification for mixtures and used evaluation method according to Regulation (EC) No 1272/2008 [CLP]

Classification	Classification procedure
Aquatic Chronic 3; H412	Calculation method

Relevant H and EUH statements (number and full text)

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H411 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.

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