

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:	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:

1

# **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.

### 3.2. Mixtures

Sum formula:	C13 H20 O
Molecular weight:	192,30 g/mol



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### **Relevant ingredients**

CAS No	Chemical name			
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
127-41-3	3 NATURAL ALPHA-IONONE			95,0 - 99,0%
	204-841-6			
14901-07-6	6 NATURAL BETA-IONONE			
	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	EC No Chemical name				
	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	238-969-9 NATURAL BETA-IONONE				
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 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/m³		
Worker DNEL,	long-term	dermal	systemic	0,28 mg/kg bw/day		
Consumer DNE	EL, long-term	inhalation	systemic	0,174 mg/m³		
Consumer DNE	EL, long-term	dermal	systemic	0,1 mg/kg bw/day		
Consumer DNE	EL, 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 <sup>3</sup>		
Worker DNEL, long-term		dermal	systemic	2,191 mg/kg bw/day		
Consumer DNE	EL, long-term	inhalation	systemic	0,621 mg/m³		
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				
Environmenta	Value				
127-41-3	127-41-3 NATURAL ALPHA-IONONE				
Freshwater 0,0034 mg/					
Marine water		0,0003 mg/l			
Freshwater s	ediment	0,984 mg/kg			
Marine sedim	nent	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 (i	intermittent releases)	0,015 mg/l			
Marine water		0 mg/l			
Freshwater s	ediment	22,451 mg/l			
Marine sedim	nent	22,451 mg/l			
Micro-organis	0,043 mg/l				
Soil	Soil				

# 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 Colour:	l state:	Liquid	
			Test method
Melting	point/freezing point:	-16 °C	
Boiling p	point or initial boiling point and	237 °C	
boiling r	ange:		
Flamma	bility:	not determined	
Lower e	xplosion limits:	not determined	
Upper e	xplosion limits:	not determined	
Flash po	pint:	87 °C	
Auto-ign	ition temperature:	not determined	
Decomp	osition temperature:	not determined	
pH-Valu	e (at 29 °C):	4,55	OECD 122
Viscosity	y / kinematic:	41,15 mm²/s	
(at 20 <sup>°</sup>	C)		
Water se	•	0,059 g/l	
(at 25 °			
Solubilit	y in other solvents		
	determined		
	coefficient n-octanol/water:	3,896	
	pressure:	0,0013 hPa	
(at 20 °	,	0.00	
	(at 20 °C):	0,93 g/cm <sup>3</sup>	
(at 20 °	vapour density:	7	
	characteristics:	not applicable	
9.2. Other i		not applicable	
	tion with regard to physical haz	zard classes	
•	e properties		
	product is not: Explosive. not exp g properties	biosive according to EU A. 14	
	product is not: oxidising.		
	afety characteristics		
-	ition rate:	not determined	
	content:	0%	
Solid co		0% 26.45 mDo o	
viscosity (at 20 °	y / dynamic:	36,45 mPa·s	
(at 20	0)		

# **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-IONO	NE			-	
	oral	LD50 mg/kg	4590	Rat	REACH Dossier	
	dermal	LD50 mg/kg	>5000	Rabbit	REACH Dossier	
14901-07-6	NATURAL BETA-IONON	E				
	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-IONON	E					
	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)

14.1. UN number or ID number:14.2. UN proper shipping name:14.3. Transport hazard class(es):14.4. Packing group:

#### Inland waterways transport (ADN)

14.1. UN number or ID number:

14.2. UN proper shipping name:

14.3. Transport hazard class(es):

14.4. Packing group:

No dangerous good in sense of these transport regulations. No dangerous good in sense of these transport regulations. No dangerous good in sense of these transport regulations.

No dangerous good in sense of these transport regulations.

No dangerous good in sense of these transport regulations. No dangerous good in sense of these transport regulations. No dangerous good in sense of these transport regulations. No dangerous good in sense of these transport regulations.



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14.1. UN number or ID number:	No dangerous good in sense of these transport regulations.			
14.2. UN proper shipping name:	No dangerous good in sense of these transport regulations.			
14.3. Transport hazard class(es): Segregation group:	No dangerous good in sense of these transport regulations. 1 - acids			
Air transport (ICAO-TI/IATA-DGR)				
14.1. UN number or ID number:	No dangerous good in sense of these transport regulations.			
14.2. UN proper shipping name:	No dangerous good in sense of these transport regulations.			
14.3. Transport hazard class(es):	No dangerous good in sense of these transport regulations.			
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 rec	gulations/legislation specific for the substance or mixture			
EU regulatory information				
Restrictions on use (REACH, annex XVI	I):			
Entry 3				
Directive 2004/42/EC on VOC in	97,5 % (906,75 g/l)			
paints and varnishes:				
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): 1,14,15.



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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 DNFL: Derived No Effect Level DMFL: 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.)