

## Safety Data Sheet

according to UN GHS (ST/SG/AC.10/11/Rev.9)

### NATURAL METHYL HEXYL KETONE (2-OCTANONE)

Revision date: 09.08.2023

Product code: 280200WW

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

##### 1.1. Product identifier

NATURAL METHYL HEXYL KETONE (2-OCTANONE)

Substance name: NATURAL METHYL HEXYL KETONE (2-OCTANONE)  
 CAS No: 111-13-7

##### 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 37
e-mail:	andreas.goertz@axxence.com	
Internet:	www.axxence.de	
Responsible Department:	QM - Regulatory Affairs	

##### 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.9)

Flammable liquid: Flam. Liq. 3  
 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 3  
 Hazardous to the aquatic environment: Aquatic Chronic 3

##### 2.2. Label elements

###### UN GHS (ST/SG/AC.10/11/Rev.9)

Signal word: Warning

Pictograms:



###### Hazard statements

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H313	May be harmful in contact with skin.
H319	Causes serious eye irritation.
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.
P233	Keep container tightly closed.

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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.
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.
P302+P317	IF ON SKIN: Get medical help.
P303+P361+P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
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.
P370+P378	In case of fire: Use Carbon dioxide (CO <sub>2</sub> ), Foam, Extinguishing powder. to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container to .

#### 2.3. Other hazards

This substance has been listed as SVHC (substance of very high concern) in the Candidate List according to Article 59 of REACH.

This substance is identified as SVHC (substance of very high concern) and is subject to authorisation according to Annex XIV of REACH.

### SECTION 3: Composition/information on ingredients

#### 3.1. Substances

Sum formula:	C <sub>8</sub> H <sub>16</sub> O
Molecular weight:	128,21

#### **Hazardous components**

CAS No	Chemical name	Quantity
	Classification (UN GHS (ST/SG/AC.10/11/Rev.9))	
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)	100 %
	Flam. Liq. 3, Acute Tox. 4, Acute Tox. 5, Eye Irrit. 2, Aquatic Acute 3, Aquatic Chronic 3; H226 H302 H313 H319 H402 H412	

### 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 (CO<sub>2</sub>), Foam, Extinguishing powder.

##### **Unsuitable extinguishing media**

Water.

#### **5.2. Special hazards arising from the substance or mixture**

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.

Suitable gloves type: -

##### 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:	colourless	
Melting point/freezing point:		-19 °C
Boiling point or initial boiling point and boiling range:		171 °C
Flammability:		not determined
Lower explosion limits:		not determined
Upper explosion limits:		not determined
Flash point:		56 °C
Auto-ignition temperature:		295 °C
Decomposition temperature:		not determined
pH-Value (at 27 °C):		4,62

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Viscosity / kinematic: (at 40 °C)	13,36 mm <sup>2</sup> /s
Water solubility: (at 20 °C)	0,9 g/L
Solubility in other solvents not determined	
Partition coefficient n-octanol/water:	2,37
Vapour pressure: (at 25 °C)	<1,8 hPa
Vapour pressure: (at 50 °C)	8,47 hPa
Density (at 20 °C):	0,82 g/cm <sup>3</sup>
Relative vapour density: (at 20 °C)	4,42

#### **9.2. Other information**

##### **Information with regard to physical hazard classes**

###### Explosive properties

The product is not: Explosive.

###### 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) 11,69 mPa·s

## SECTION 10: Stability and reactivity

### **10.1. Reactivity**

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.

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CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)				
	oral	LD50 mg/kg	<2000	Rat	REACH registration OECD 423
	dermal	LD50 mg/kg	>2000	Rat	REACH registration OECD 402

#### Irritation and corrosivity

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

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

This substance is classified as hazardous according to Regulation (EC) No 1272 (2008).

### SECTION 12: Ecological information

#### 12.1. Toxicity

Harmful to aquatic life with long lasting effects.

CAS No	Chemical name					
	Aquatic toxicity	Dose	[h]   [d]	Species	Source	Method
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)					
	Acute fish toxicity	LC50 mg/l	45,9	96 h	Pimephales promelas (fathead minnow)	REACH registration
	Acute algae toxicity	ErC50 mg/l	>100	72 h	Desmodesmus subspicatus	REACH registration OECD 201
	Acute crustacea toxicity	EC50 mg/l	59,6	48 h	Daphnia magna (Big water flea)	REACH registration OECD 202
	Acute bacteria toxicity	(EC50 mg/l)	>10	0,5 h		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			
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)			
	OECD 301 D	45%	35	
	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
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)	2,37

#### **BCF**

CAS No	Chemical name	BCF	Species	Source
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)	13	-	REACH DOssier

#### **12.4. Mobility in soil**

The product has not been tested.

#### **12.6. Endocrine disrupting properties**

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

No information available.

#### **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.

##### **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)**

<b>14.1. UN number or ID number:</b>	UN 1224
<b>14.2. UN proper shipping name:</b>	KETONES, LIQUID, N.O.S.
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3



Special Provisions:	223 274
Limited quantity:	5 L
Excepted quantity:	E1

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EmS: F-E, S-D

#### Air transport (ICAO-TI/IATA-DGR)

<b>14.1. UN number or ID number:</b>	UN 1224
<b>14.2. UN proper shipping name:</b>	KETONES, LIQUID, N.O.S.
<b>14.3. Transport hazard class(es):</b>	3
<b>14.4. Packing group:</b>	III
Hazard label:	3



Special Provisions:	A3	
Limited quantity Passenger:	10 L	
Passenger LQ:	Y344	
Excepted quantity:	E1	
IATA-packing instructions - Passenger:		355
IATA-max. quantity - Passenger:		60 L
IATA-packing instructions - Cargo:		366
IATA-max. quantity - Cargo:		220 L

#### 14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

#### 14.6. Special precautions for user

Warning: Combustible liquid.

#### 14.7. Maritime transport in bulk according to IMO instruments

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

#### 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%



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