

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL METHYL HEXYL KETONE (2-OCTANONE)

Revision date: 09.08.2023

Product code: 280200

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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
EC No: 203-837-1

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
E-mail: info@axxence.com
Contact person: Safety Team
E-mail: safety-documentation@axxence.com
Internet: www.axxence.de
Responsible Department: Safety Management

Telefax: + 49 2822 68561 39

Telephone: + 49 2822 68561 0

1.4. Emergency telephone

+49 2822 68561 99

number:

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Flam. Liq. 3; H226
Acute Tox. 4; H302
Eye Irrit. 2; H319
Aquatic Chronic 3; H412

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word: Warning

Pictograms:



Hazard statements

H226 Flammable liquid and vapour.
H302 Harmful if swallowed.
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.
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+P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P330	Rinse mouth.
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+P313	If eye irritation persists: Get medical advice/attention.
P370+P378	In case of fire: Use Carbon dioxide (CO ₂), Foam, Extinguishing powder. to extinguish.
P403+P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/container to organic waste.

2.3. Other hazards

This substance is not listed as Substance of Very High Concern (SVHC) in the Candidate List according to REACH, Article 59.

This substance is not identified as SVHC (substance of very high concern) and is not subject to authorisation according to Annex XIV of REACH.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C ₈ H ₁₆ O
Molecular weight:	128,21 g/mol

Relevant ingredients

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (Regulation (EC) No 1272/2008)			
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)			100 %
	203-837-1			
	Flam. Liq. 3, Acute Tox. 4, Eye Irrit. 2, Aquatic Chronic 3; H226 H302 H319 H412			

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	
111-13-7	203-837-1	NATURAL METHYL HEXYL KETONE (2-OCTANONE)	100 %
	dermal: LD50 = >2000 mg/kg; oral: LD50 = <2000 mg/kg		

SECTION 4: First aid measures

4.1. Description of first aid measures

After inhalation

Provide fresh air.

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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.

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

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

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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.

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.

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

DNEL/DMEL values

CAS No	Name of agent			
DNEL type	Exposure route	Effect	Value	
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)			
Worker DNEL, long-term	inhalation	systemic	1580 mg/m ³	
Worker DNEL, long-term	dermal	systemic	3 mg/kg bw/day	
Consumer DNEL, long-term	inhalation	systemic	281 mg/m ³	
Consumer DNEL, long-term	dermal	systemic	0,357 mg/kg bw/day	
Consumer DNEL, long-term	oral	systemic	0,0167 mg/kg bw/day	

PNEC values

CAS No	Name of agent		
Environmental compartment	Value		
111-13-7	NATURAL METHYL HEXYL KETONE (2-OCTANONE)		
Freshwater			0,05 mg/l
Marine water			0,005 mg/l
Freshwater sediment			0,464 mg/kg
Marine sediment			0,05 mg/kg
Soil			0,066 mg/kg

8.2. Exposure controls

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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
Viscosity / kinematic: (at 40 °C)	13,36 mm²/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/cm³
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.

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Oxidizing properties

The product is not: oxidising.

Other safety characteristics

Evaporation rate:

not determined

Solvent content:

0%

Solid content:

0%

Viscosity / dynamic:

11,69 mPa·s

(at 20 °C)

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 hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

Harmful if swallowed.

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

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.

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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
	Acute crustacea toxicity	EC50 mg/l	59,6	48 h	Daphnia magna (Big water flea)	REACH registration
	Acute bacteria toxicity	EC50 ()	>10 mg/l	0,5 h		REACH registration

12.2. Persistence and degradability

The product has not been tested.

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.

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

The product has not been tested.

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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.

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: UN 1224
14.2. UN proper shipping name: KETONES, LIQUID, N.O.S.
14.3. Transport hazard class(es): 3
14.4. Packing group: III
Hazard label: 3



Classification code: F1
Special Provisions: 274
Limited quantity: 5 L
Excepted quantity: E1
Transport category: 3
Hazard No: 30
Tunnel restriction code: D/E

Other applicable information (land transport)

E1

Inland waterways transport (ADN)

14.1. UN number or ID number: UN 1224
14.2. UN proper shipping name: KETONES, LIQUID, N.O.S.

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14.3. Transport hazard class(es):

3

14.4. Packing group:

III

Hazard label:

3



Classification code:

F1

Special Provisions:

274

Limited quantity:

5 L

Excepted quantity:

E1

Other applicable information (inland waterways transport)

E1

Marine transport (IMDG)

14.1. UN number or ID number:

UN 1224

14.2. UN proper shipping name:

KETONES, LIQUID, N.O.S.

14.3. Transport hazard class(es):

3

14.4. Packing group:

III

Hazard label:

3



Special Provisions:

223 274

Limited quantity:

5 L

Excepted quantity:

E1

EmS:

F-E, S-D

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number:

UN 1224

14.2. UN proper shipping name:

KETONES, LIQUID, N.O.S.

14.3. Transport hazard class(es):

3

14.4. Packing group:

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

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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, Entry 40

Directive 2010/75/EU on industrial emissions: 100 % (820 g/l)

Directive 2004/42/EC on VOC in paints and varnishes: 100 % (820 g/l)

Information according to Directive 2012/18/EU (SEVESO III): P5c FLAMMABLE LIQUIDS

Additional information

To follow: 850/2004/EC, 79/117/EEC, 689/2008/EC

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): 1 - slightly hazardous to water

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Changes

This data sheet contains changes from the previous version in section(s): 1,2,4,5,6,7,8,9,11,12,13,14,15,16.

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Abbreviations and acronyms

Flam. Liq: Flammable liquid
 Acute Tox: Acute toxicity
 Eye Irrit: Eye irritation
 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>
 For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety
 assessment, chapter R.20 (Table of terms and abbreviations).

Relevant H and EUH statements (number and full text)

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
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.

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