

according to Regulation (EC) No 1907/2006

NATURAL 4-METHYLPENTANOIC ACID

Revision date: 17.02.2025

Product code: 346300

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

1.1. Product identifier

NATURAL 4-METHYLPENTANOIC ACID

Substance name:	NATURAL 4-METHYLPENTANOIC ACID
CAS No:	646-07-1
EC No:	211-464-0

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:

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Skin Corr. 1C; H314 Eye Dam. 1; H318

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Signal word:	Danger
olgilal word.	Danger

Pictograms:



Hazard statements

H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
Precautionary statemen	Its
P260	Do not breathe dust/fume/gas/mist/vapours/spray.
P264	Wash thoroughly after handling.
P280	Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
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

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	present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER/doctor.
P321	Specific treatment (see on this label).

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 identifed as SVHC (substance of very high concern) and is not subject to autorisation according to Annex XIV of REACH.

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula:	C6 H12 O2
Molecular weight:	116,1578 g/mol

Relevant ingredients

CAS No	Chemical name			Quantity		
	EC No	EC No Index No REACH No				
	Classification (Regulation (EC) No 1272/2008)					
646-07-1	NATURAL 4-METHYLPENTANOIC ACID					
	211-464-0					
	Skin Corr. 1C, Eye Dam. 1; H314 H	Skin Corr. 1C, Eye Dam. 1; H314 H318				

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. L	imits, M-factors and ATE				
646-07-1	211-464-0 NATURAL 4-METHYLPENTANOIC ACID					
	dermal: LD50 = 968 mg/kg; oral: LD50 = 2050 mg/kg					

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down.

After inhalation

Provide fresh air. Medical treatment necessary.

After contact with skin

After contact with skin, wash immediately with plenty of water and soap. Take off immediately all contaminated clothing and wash it before reuse. If skin irritation occurs: Get medical advice/attention.

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink 1 glass of of water. Do NOT induce vomiting. Adverse human health effects and symptoms: Gastric perforation. Call a physician immediately. Do not allow a neutralisation agent to be drunk.

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.



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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

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

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

Provide adequate ventilation. 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 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.

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

No special fire protection measures are necessary.

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.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaustion at critical locations.

Hints on joint storage

No special measures are necessary.

7.3. Specific end use(s)



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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

8.2. Exposure controls



Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe gas/fumes/vapour/spray.

Individual protection measures, such as personal protective equipment

Eye/face protection

Suitable eye protection: goggles.

Hand protection

Suitable gloves type: Butyl caoutchouc (butyl rubber) / FKM (fluoro rubber).

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.

Recommended material: Butyl caoutchouc (butyl rubber), FKM (fluoro rubber)

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:		
Melting point/freezing point:		No data available
Boiling point or initial boiling point and		199-201 °C
boiling range:		
Flammability:		No data available
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		97,2 °C
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic:		No data available
Water solubility:		easily soluble
Solubility in other solvents		
not determined		
Partition coefficient n-octanol/water:		No data available
Vapour pressure:		No data available



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0,92 g/cm³

No data available

No data available

not applicable

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Density (at 25 °C): Relative vapour density: Particle characteristics:

9.2. Other information

Information with regard to physical hazard classes Explosive properties The product is: not explosive according to EU A.14 Sustaining combustion: Oxidizing properties The product is not: oxidising.

SECTION 10: Stability and reactivity

10.1. Reactivity

No hazardous reaction when handled and stored according to provisions.

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.

CAS No	Chemical name						
	Exposure route	Dose		Species	Source	Method	
646-07-1	NATURAL 4-METHYLPENTANOIC ACID						
	oral	LD50 205 mg/kg	50	Rat			
	dermal	LD50 968 mg/kg	8	Rabbit			

Irritation and corrosivity

Skin corrosion/irritation: Causes severe skin burns and eye damage. Serious eye damage/eye irritation: Causes serious eye damage.

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.

Other information

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

SECTION 12: Ecological information

12.1. Toxicity

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

CAS No	Chemical name						
	Aquatic toxicity	Dose		[h] [d]	Species	Source	Method
646-07-1	NATURAL 4-METHYLPE	NTANOIC	ACID				
	Acute fish toxicity	LC50	88 mg/l		Pimephales promelas (fathead minnow)		
	Acute algae toxicity	ErC50 mg/l	56,4		Pseudokirchneriella subcapitata		
	Acute crustacea toxicity	EC50	72 mg/l		Daphnia magna (Big water flea)		
	Crustacea toxicity	NOEC mg/l	17,9		Daphnia magna (Big water flea)		

12.2. Persistence and degradability

The product has not been tested.

12.3. Bioaccumulative potential

The product has not been tested.

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
646-07-1	NATURAL 4-METHYLPENTANOIC ACID	1.56

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.

12.6. Endocrine disrupting properties

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

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



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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 2922
14.2. UN proper shipping name:	CORROSIVE LIQUID, TOXIC, N.O.S.
<u>14.3. Transport hazard class(es):</u>	8
14.4. Packing group:	III
Hazard label:	8+6.1
	6
Classification code:	CT1
Special Provisions:	274
Limited quantity:	5 L
Excepted quantity:	E1
Transport category:	3
Hazard No:	86
Tunnel restriction code:	E
Inland waterways transport (ADN)	
14.1. UN number or ID number:	UN 2922
14.2. UN proper shipping name:	CORROSIVE LIQUID, TOXIC, N.O.S.
14.3. Transport hazard class(es):	8
14.4. Packing group:	111
Hazard label:	8+6.1
	Â.
	8 6
Classification code:	CT1 Č
Special Provisions:	274 802
Limited quantity:	5 L
Excepted quantity:	E1
Marine transport (IMDG)	
14.1. UN number or ID number:	UN 2922
14.2. UN proper shipping name:	CORROSIVE LIQUID, TOXIC, N.O.S.
14.3. Transport hazard class(es):	8
14.4. Packing group:	III

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Hazard label:	8+6.1	
Special Provisions: Limited quantity: Excepted quantity: EmS:	223 274 5 L E1 F-A, S-B	
Air transport (ICAO-TI/IATA-DGR) <u>14.1. UN number or ID number:</u> <u>14.2. UN proper shipping name:</u> <u>14.3. Transport hazard class(es):</u> <u>14.4. Packing group:</u> Hazard label:	UN 2922 CORROSIVE LIQUID, TOXIC, N.O.S. 8 III 8+6.1	
Special Provisions: Limited quantity Passenger: Passenger LQ: Excepted quantity: IATA-packing instructions - Passenger: IATA-max. quantity - Passenger: IATA-packing instructions - Cargo: IATA-max. quantity - Cargo:	A3 A4 A803 1 L Y841 E1 852 5 L 856 60 L	
14.5. Environmental hazards		
ENVIRONMENTALLY HAZARDOUS:	No	
 14.6. Special precautions for user Warning: strongly corrosive. 14.7. Maritime transport in bulk according to not applicable 	o IMO instruments	
SECTION 15: Regulatory information		
15.1. Safety, health and environmental regul	ations/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:	95 % (874 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 'juveni work protection guideline' (94/33/EC).	le
Water hazard class (D):	3 - highly hazardous to water	

15.2. Chemical safety assessment

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

SECTION 16: Other information



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Abbreviations and acronyms

Skin Corr: Skin corrosion Eye Dam: Eye damage 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** EC/EEC: European Community/European Economic Community EU: European Union CAS: Chemical Abstracts Service DNEL: Derived No Effect Level DMEL: Derived Minimal Effect Level PNEC: Predicted No Effect Concentration ATE: Acute toxicity estimate LC50: Lethal concentration, 50% LD50: Lethal dose, 50% 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 M-factor: Multiplying factor ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road) 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) IMDG: International Maritime Code for Dangerous Goods EmS: Emergency Schedules MFAG: Medical First Aid Guide IATA: International Air Transport Association DGR: Dangerous Goods Regulations ICAO: International Civil Aviation Organization TI: Technical Instructions MARPOL: International Convention for the Prevention of Marine Pollution from Ships IBC: Intermediate Bulk Container VOC: volatile organic compound SVHC: Substance of Very High Concern

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)

- H314 Causes severe skin burns and eye damage.
- H318 Causes serious eye damage.

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.