

Safety Data Sheet

according to Regulation (EC) No 1907/2006

NATURAL ISOBUTYL HEXANOATE (CAPROATE)

Revision date: 23.09.2022

Product code: 220200

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
105-79-3	203-332-6	NATURAL ISOBUTYL HEXANOATE (CAPROATE)	100 %
		oral: LD50 = >5000 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

Observe risk of aspiration if vomiting occurs. Rinse mouth immediately and drink 1 glass of water. Rinse mouth immediately and drink plenty 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.

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.

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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****8.2. Exposure controls****Individual protection measures, such as personal protective equipment****Eye/face protection**

Wear eye/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 supplier of these gloves. Suitable gloves type: Butyl caoutchouc (butyl rubber)

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	Liquid	
Colour:	colourless	
Odour:	fruity	
Melting point/freezing point:		not determined
Boiling point or initial boiling point and boiling range:		177 °C
Flammability		
Solid/liquid:		not applicable
Gas:		not applicable
Lower explosion limits:		not determined
Upper explosion limits:		not determined
Flash point:		76 °C
Auto-ignition temperature:		not determined
Decomposition temperature:		not determined
pH-Value:		not determined
Water solubility: (at 20 °C)		0,039 g/L
Solubility in other solvents		
not determined		
Partition coefficient n-octanol/water:		3,686
Vapour pressure:		not determined
Density (at 20 °C):		0,86 g/cm ³
Relative vapour density: (at 20 °C)		5,9

9.2. Other information

Information with regard to physical hazard classes

- Explosive properties
 - 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%

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.

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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
105-79-3	NATURAL ISOBUTYL HEXANOATE (CAPROATE)				
	oral	LD50 >5000 mg/kg	Rat	Moreno, 1975b	

Irritation and corrosivity

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

The substance is classified as not hazardous according to regulation (EC) No 1272/2008 [CLP].

SECTION 12: Ecological information**12.1. Toxicity**

The product is not: Ecotoxic.

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
105-79-3	NATURAL ISOBUTYL HEXANOATE (CAPROATE)	3,686

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.

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

160306 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes other than those mentioned in 16 03 05

List of Wastes Code - used product

160306 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; off-specification batches and unused products; organic wastes other than those mentioned in 16 03 05

List of Wastes Code - contaminated packaging

150102 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); plastic packaging

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)

<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: No

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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

2004/42/EC (VOC):	100 % (860 g/l)
Information according to 2012/18/EU (SEVESO III):	Not subject to 2012/18/EU (SEVESO III)

Additional information

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

National regulatory information

Water hazard class (D): 2 - obviously 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): 1,2,3,4,5,6,7,8,9,11,13,14,15,16.

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%

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)

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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.