

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND THE COMPANY/UNDERTAKING

1.1. Identification of the substance/mixture

Trade name: KOHINOOL® IFF
Substance name: 3,4,5,6,6-PENTAMETHYLHEPTAN-2-OL
CAS Number: 87118-95-4
CE Number: 401-030-0

1.2. Relevant identified uses of the substance or mixture and uses advised against

Raw material for the manufacture of fragrances and/or flavourings.

1.3. Details of the supplier of the safety data sheet

Company: Ernesto Ventós SA
Address: Carretera Real, 120 B
08960 Sant Just Desvern – Barcelona – SPAIN
Telephone: (00 34) 934 706 210
Fax: (00 34) 934 733 010
E-mail: info@ventos.com

1.4. Emergency telephone number

NCEC (+44) 1865 407333 (24h)
NCEC (+34) 91 114 2520 (24h) (ES)
NCEC (+1) 202 464 2554 (24h) (USA, Canada)

2. HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

Flammable Liquids - Category 4 - H227
Hazardous to the aquatic environment, short-term (acute) - Category 2 - H401
Hazardous to the aquatic environment, long-term (chronic) - Category 2 - H411

2.2. Label Elements

Hazard pictograms:



Signal Word:
Warning

Hazard statements:

H227 – Combustible liquid.
H411 – Toxic to aquatic life with long lasting effects.

Precautionary statements:

P210 – Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P273 – Avoid release to the environment.
P280 – Wear protective gloves/protective clothing/eye protection/face protection.
P370+P378 – In case of fire: Use carbon dioxide, foam, dry powder or water spray for extinction.
P391 – Collect spillage.
P403 – Store in a well-ventilated place.

2.3. Other hazards

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Chemical name: 3,4,5,6,6-PENTAMETHYLHEPTAN-2-OL
CAS number: 87118-95-4
EC number: 401-030-0

Hazardous constituents:

Chemical Name	% (w/w)	CAS No. EC No.	Classification according to GHS
3,4,5,6,6-PENTAMETHYLHEPTAN-2-OL	≥50	87118-95-4 401-030-0	Flammable Liquids - Category 4 - H227 Hazardous to the aquatic environment, short-term (acute) - Category 2 - H401 Hazardous to the aquatic environment, long-term (chronic) - Category 2 - H411

See the full text of the hazard statements in section 16.

3.2. Mixtures

Not applicable.

4. FIRST-AID MEASURES

4.1. Description of necessary first aid measures

Ingestion:	Rinse mouth with water. Obtain medical advice. Keep at rest. Do not induce vomiting.
Eye contact:	In case of contact with eyes, rinse immediately with plenty of water for at least 15 minutes and seek medical advice.
Inhalation:	Remove person to fresh air and keep at rest. Seek immediate medical advice.
Skin contact:	Take off immediately all contaminated clothing. Thoroughly wash affected skin with soap and water. Seek medical attention if symptoms persist.

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

No information available.

5. FIRE-FIGHTING MEASURES

5.1. Extinguishing Media

Water spray, carbon dioxide, dry chemical powder or appropriate foam.
For safety reasons do not use full water jet.

5.2. Special hazards arising from the substance or mixture

Known or Anticipated Hazardous Products of Combustion: Emits toxic fumes under fire conditions.

5.3. Advice for firefighters

High temperatures can lead to high pressures inside closed containers.
Avoid inhalation of vapors that are created. Use appropriate respiratory protection.
Do not allow spillage of fire to be poured into drains or watercourses.
Wear self-contained breathing apparatus and protective clothing.

6. ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Evacuate surrounding areas. Ensure adequate ventilation. Keep unnecessary and unprotected personnel from entering.
Do not breathe vapor/spray. Avoid contact with skin and eyes. Information regarding personal protective measures: see section 8.

6.2. Environmental precautions

To avoid possible contamination of the environment, do not discharge into any drains, surface waters or groundwaters.

6.3. Methods and materials for containment and cleaning up

Cover with an inert, inorganic, non-combustible absorbent material (e.g. dry-lime, sand, soda ash).
Place in covered containers using non-sparking tools and transport outdoors.
Avoid open flames or sources of ignition (e.g. pilot lights on gas hot water heater).
Ventilate area and wash spill site after material pickup is complete.

6.4. Reference to other sections

Information regarding exposure controls, personal protection and disposal considerations can be found in sections 8 and 13.

7. HANDLING AND STORAGE

7.1. Precautions for safe handling

Do not store or handle this material near food or drinking water. Do not smoke.
Avoid contact with the eyes, skin and clothing. Wear protective clothing and use glasses.
Observe the rules of safety and hygiene at work.
Keep in the original container or an alternative made from a compatible material.

7.2. Conditions for safe storage, including any incompatibilities

Store in tightly closed and preferably full containers in a cool, dry and ventilated area, protected from light.
Keep away from sources of ignition (e.g. hot surfaces, sparks, flame and static discharges).
Keep away from incompatible materials (see section 10).

7.3. Specific end use(s)

No information available.

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

8.1. Control parameters

Components with occupational exposure limits:
None known.

8.2. Exposure controls

Measures should be taken to prevent materials from being splashed into the body.
Provide adequate ventilation, according to the conditions of use. Use a mechanical exhaust if required.

8.3. Individual protection measures, such as personal protective equipment

Eye/Face protection:	Chemical safety goggles are recommended. Wash contaminated goggles before reuse.
Hand Protection:	Chemical-resistant gloves are recommended. Wash contaminated gloves before reuse.
Body protection:	Personal protective equipment for the body should be selected based on the task being performed and the risks involved.
Respiratory Protection:	In case of insufficient ventilation, use suitable respiratory equipment.
Environmental exposure controls:	Emissions from ventilation or process equipment should be checked to ensure they comply with environmental protection legislation. In some cases, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance:	Liquid
Colour:	Conforms to standard
Odour:	Conforms to standard
Odour threshold:	Not determined
pH:	Not determined
Melting point/freezing point:	Not determined
Boiling point/boiling range (°C):	Not determined
Flash point:	93 °C
Evaporation rate:	Not determined
Flammability:	Not determined
Lower flammability/Explosive limit:	Not determined
Upper flammability/Explosive limit:	Not determined
Vapour pressure:	0,03 mm Hg (25°C)
Vapour Density:	Not determined
Density:	0,864–0,872 g/mL (20°C)
Relative density:	0,864–0,872 (20°C)
Water solubility:	INSOLUBLE IN WATER
Solubility in other solvents:	SOLUBLE IN ETHANOL
Partition coefficient n-octanol/water:	Not determined
Auto-ignition temperature:	Not determined
Decomposition temperature:	Not determined
Viscosity, dynamic:	Not determined
Viscosity, kinematic:	Not determined
Explosive properties:	Not determined
Oxidising properties:	NONE EXPECTED

10. STABILITY AND REACTIVITY

10.1. Reactivity

No hazardous reactions if stored and handled as prescribed/indicated.

10.2. Chemical stability

The product is stable if stored and handled as prescribed/indicated.

10.3. Possibility of hazardous reactions

No hazardous reactions if stored and handled as prescribed/indicated.

10.4. Conditions to Avoid

Conditions to Avoid: Excessive heat, flame or other ignition sources.

10.5. Incompatible materials

Avoid contact with strong acids and bases and oxidizing agents.

10.6. Hazardous decomposition products

During combustion may form carbon monoxide and unidentified organic compounds.

11. TOXICOLOGICAL INFORMATION

Acute toxicity	Based on the data available, the criteria for classification are not met.
Skin corrosion/irritation	Based on the data available, the criteria for classification are not met.
Serious eye damage/irritation	Based on the data available, the criteria for classification are not met.
Respiratory or skin sensitisation	Based on the data available, the criteria for classification are not met.
Germ cell mutagenicity	Based on the data available, the criteria for classification are not met.
Carcinogenicity	Based on the data available, the criteria for classification are not met.
Reproductive toxicity	Based on the data available, the criteria for classification are not met.
STOT-single exposure	Based on the data available, the criteria for classification are not met.
STOT-repeated exposure	Based on the data available, the criteria for classification are not met.
Aspiration hazard	Based on the data available, the criteria for classification are not met.

12. ECOLOGICAL INFORMATION

12.1. Toxicity

Assessment:

Toxic to aquatic life with long lasting effects.

Experimental/calculated data:

No information available.

12.2. Persistence and degradability

The product is not readily biodegradable

12.3. Bioaccumulative potential

No information available.

12.4. Soil mobility

No information available.

12.5. Other adverse effects

See also sections 6, 7, 13 and 15

Do not allow to get into waste water or waterways.

13. DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Dispose of in accordance with national and local environmental regulations.

14. TRANSPORT INFORMATION

	ADR/RID/ADN	IMDG	IATA-ICAO
14.1. UN Number	UN3082	UN3082	UN3082
14.2. UN Proper Shipping Name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (3,4,5,6, 6-PENTAMETHYLHEPTAN-2-OL)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (3,4,5,6, 6-PENTAMETHYLHEPTAN-2-OL)	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (3,4,5,6, 6-PENTAMETHYLHEPTAN-2-OL)
14.3. Transport Hazard Class(es)	9	9	9
14.4. Packing Group	III	III	III
14.5. Environmental hazards	Yes	Yes	Yes
Additional information			

14.6 Special precautions for user

None known

14.7. Maritime transport in bulk according to IMO instruments

No information available

15. REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

No information available

16. OTHER INFORMATION

Full text of the R-phrases, hazard statements and precautionary statements mentioned in section 3:

H227 – Combustible liquid.

H401 – Toxic to aquatic life.

H411 – Toxic to aquatic life with long lasting effects.

The information included in this safety data sheet is based on the available data at the moment this document is issued. It is meant to be a description of safety requirements for our product and does not stand for a guarantee of its properties. The user is responsible for taking all necessary steps leading to compliance with local rules and legislation.