

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

### 1.1. Identification of the substance/mixture

**Trade name:** IRISONE PCAS  
**Substance name:** 4-TERT-BUTYLCICLOHEXANONE  
**CAS Number:** 98-53-3  
**CE Number:** 202-678-5

### 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

Acute Toxicity - Category 4 (oral) - H302  
Hazardous to the aquatic environment, short-term (acute) - Category 3 - H402  
Hazardous to the aquatic environment, long-term (chronic) - Category 3 - H412

### 2.2. Label Elements

**Hazard pictograms:**



**Signal Word:**  
Warning

#### **Hazard statements:**

H302 – Harmful if swallowed.  
H412 – Harmful to aquatic life with long lasting effects.

#### **Precautionary statements:**

P264 – Wash thoroughly after handling.  
P270 – Do not eat, drink or smoke when using this product.  
P273 – Avoid release to the environment.  
P301+P312+P330 – IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.  
P501 – Dispose of contents/container according to local legislation.

### 2.3. Other hazards

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1. Substances

**Chemical name:** 4-TERT-BUTYLCICLOHEXANONE  
**CAS number:**  
**EC number:** 202-678-5

**Hazardous constituents:**

Chemical Name	% (w/w)	CAS No. EC No.	Classification according to GHS
4-TERT-BUTYLCYCLOHEXANONE	≥50	98-53-3 202-678-5	Acute Toxicity - Category 4 (oral) - H302 Acute Toxicity - Category 5 (dermal) - H313 Hazardous to the aquatic environment, short-term (acute) - Category 3 - H402 Hazardous to the aquatic environment, long-term (chronic) - Category 3 - H412

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:	Solid
Colour:	Conforms to standard
Odour:	Conforms to standard
Odour threshold:	Not determined
pH:	Not determined
Melting point/freezing point:	48 APROX.
Boiling point/boiling range (°C):	Not determined
Flash point:	89 °C
Evaporation rate:	Not determined
Flammability:	Not determined
Lower flammability/Explosive limit:	Not determined
Upper flammability/Explosive limit:	Not determined
Vapour pressure:	Not determined
Vapour Density:	Not determined
Density:	Not determined
Relative density:	Not determined
Water solubility:	SOLUBILITY IN WATER: 0,59 g/l (20°C)
Solubility in other solvents:	SOLUBLE IN ETHANOL
Partition coefficient n-octanol/water:	log Pow 2,6
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

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

## 12. ECOLOGICAL INFORMATION

### 12.1. Toxicity

#### Assessment:

Harmful 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
<b>14.1. UN Number</b>	Not classified as hazardous goods	Not classified as hazardous goods	Not classified as hazardous goods
<b>14.2. UN Proper Shipping Name</b>	Not applicable	Not applicable	Not applicable
<b>14.3. Transport Hazard Class(es)</b>	Not applicable	Not applicable	Not applicable
<b>14.4. Packing Group</b>	Not applicable	Not applicable	Not applicable
<b>14.5. Environmental hazards</b>	No	No	No
<b>Additional information</b>			

#### 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:

H302 – Harmful if swallowed.

H313 – May be harmful in contact with skin.

H402 – Harmful to aquatic life.

H412 – Harmful 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.