



# Safety Data Sheet

Printed : 07/04/2020

Revised : V1-R-1-CLP from 07/04/2020

## ISORALDEINE CETONE ALPHA

### 1. SECTION 1 - IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY

#### 1.1. Product identifier

Name of the substance/mixture : ISORALDEINE CETONE ALPHA

N° CAS TSCA : 1335-46-2

N° CE : 215-635-0 ; 204-846-3

N° index REACH An VI : /

N° REACH (partially) : 01-2120745133-63-xxxx

Chemical / REACH name : 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one

Molecular formula : C<sub>14</sub> H<sub>22</sub> O

Molecular weight : 206.3

IUPAC Name : 3-Methyl-4-(2,6,6-trimethyl-2-cyclohexenyl)-3-buten-2-one; Methyl-gamma-ionone; gamma-Methylionone

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

Use of the substance/mixture : Industrial use only

End use : Fragrances / Cosmetic

#### 1.3. Details of the supplier of the safety data sheet

SAS PCW

Aromagrasse - 45 bd Marcel Pagnol

06130 Grasse - FRANCE

Tel : +33 (0)4 92 42 35 00

Fax : +33 (0)4 92 42 35 19

Web : [www.pcwfrance.com](http://www.pcwfrance.com)

Email : [info@pcwfrance.com](mailto:info@pcwfrance.com)

Technical manager : [regulatory@pcwfrance.com](mailto:regulatory@pcwfrance.com)

#### 1.4. Emergency telephone number

Emergency information service of the company

+33(6) 07 85 74 60 (24h/24h)

National emergency information service

INERIS : +33(8) 20 20 18 16

Anti poison Centers in France

ORFILA : +33(1) 45 42 59 59

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## 2. SECTION 2 - HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### GHS Classification :

(RegulationCLP)

Aquatic Chronic 2 Hazardous to the aquatic environment, long-term hazard 2  
Skin Irrit. 2 Skin corrosion / irritation 2  
Skin. Sens. 1 Sensitisation skin 1

H315 - Causes skin irritation.

H317 - May cause an allergic skin reaction.

H411 - Toxic to aquatic life with long lasting effects.

### 2.2. Label elements

#### GHS Classification :

(RegulationCLP)



Warning mention : Warning

Aquatic Chronic 2 Hazardous to the aquatic environment, long-term hazard 2  
Skin Irrit. 2 Skin corrosion / irritation 2  
Skin. Sens. 1 Sensitisation skin 1

H315 - Causes skin irritation.

H317 - May cause an allergic skin reaction.

H411 - Toxic to aquatic life with long lasting effects.

P261 - Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 - Contaminated work clothing should not be allowed out of the workplace.

P280 - Wear protective gloves/protective clothing/eye protection/face protection.

P302+P352 - IF ON SKIN: Wash with plenty of soap and water.

P333+P313 - If skin irritation or rash occurs: Get medical advice/attention.

P362+P364 - Take off contaminated clothing and wash it before reuse.

P501 - Dispose of contents/container according to the local/ regional / national / international Regulation.

### 2.3. Other hazards

**Contains Alpha-Isomethyl ionone**

PBT :

**This substance is not considered as persistent, neither bioaccumulable nor toxin**

vPvB :

**This substance is not considered as very persistent nor very bioaccumulative**

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VOC Swiss - Annex 1 : **Not listed**

LVP-VOC / INORGANIC / EXEMPTED **100%**

VOC (CARB) :

CMR (Reg. 1223/2009/EEC) : **See certificate**

## 3. SECTION 3 - COMPOSITION INFORMATION ON INGREDIENTS

### 3.1. Substances

Material	C.A.S	EINECS	Classification	Percent %
Alpha-Isomethyl ionone (Regist. : /)	127-51-5	204-846-3	Aquatic Chronic 2, Skin Irrit. 2, Skin. Sens. 1B - H315, H317, H319, H320, H411	> 50 %

### 3.2. Mixtures

NO CONCERNED

## 4. SECTION 4 - FIRST AID MEASURES

### 4.1. Description of first aid measures

**General notes** : Please refer to the risk and safety statements (section 2)

**Following inhalation** : If inhaled : If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Remove collar, belt, tie... Give artificial respiration if not breathing.

**Following ingestion** : If swallowed: Immediately call a POISON CENTER or doctor/physician. Rinse mouth. Do NOT induce vomiting.

**Following skin contact** : If on skin (or hair) or clothing rinse immediately contaminated clothing and skin with plenty of water before removing clothes. If the symptom persists, consult a doctor.

**Following eye contact** : Rinse cautiously with water for several minutes (15 minutes open eyelids). Remove contact lenses, if present and easy to do. Continue rinsing. In case of disorder, consult an ophthalmologist.

**Self-protection of the first aider** : In lack of appropriate formation, none initiative should imply an individual risk.

### 4.2. Most important symptoms and effects, both acute and delayed

See section 2

### 4.3. Indication of any immediate medical attention and special treatment needed

See section 2

## 5. SECTION 5 - FIREFIGHTING MEASURES

### 5.1. Extinguishing media

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**Suitable extinguishing media :** Use an extinguishing agent suitable for the surrounding fire. CO<sub>2</sub>, powder, foam, specific liquid.

**Unsuitable extinguishing media :** Never use a direct stream of water.

## 5.2. Special hazards arising from the substance or mixture

**Flammability :** The product is not flammable.

**Prevention :** Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

**Particular risks linked to exposure :** see section 2

### Hazardous combustion products :

Release of poison gases : Monoxide de carbone (CO), Dioxyde de carbon (CO<sub>2</sub>), Oxyde d'azotes (NO<sub>x</sub>), Dioxyde de soufre (SO<sub>2</sub>), Cyanures (CN) ....

Auto-ignition temperature (°C) : **260**

## 5.3. Advice for firefighters

**Fire-fighting equipment :** use an appropriate personal protective equipment with an approved positive-pressure self-contained breathing apparatus.

## 6. SECTION 6 - ACCIDENTAL RELEASE MEASURES

### 6.1. Personal precautions, protective equipment and emergency procedures

Call immediately the emergency personnel.

Promote adequate ventilation in the area.

#### For non-emergency personnel

Keep them away from the area. Avoid all sources of ignition (spark or flame).

Avoid skin/eye contact. Do not inhale vapours.

#### For emergency responders

Use personal protective equipment. In case of accidental spills, wear protective gloves during the handling.

### 6.2. Environmental precautions

Avoid the dispersion and flow of the product. Keep away from drains, surface and ground water.

Inform the competent authorities if the product enters in ground or surface waters.

### 6.3. Methods and material for containment and cleaning up

#### For containment

The spillage is contained with sand or inert powder. The chemical waste is placed in sealed containers.

#### For cleaning up

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The soiled elements (rags, absorbent papers, filters) are immediately soaked into water. The chemical waste are rapidly treated according to the local reglementation

## Other informations

Only qualified personnel is allowed to clean up.

### **6.4. Reference to other sections**

See section 8 for personal protective equipment and section 13 for waste treatment.

## 7. SECTION 7 - HANDLING AND STORAGE

### **7.1. Precautions for safe handling**

#### Protective measures:

See section 2.2



#### Measures to prevent fire:

Do not smoke. Do not expose to excessive heat or ignition sources (spark or flame).

#### Measures to prevent aerosol and dust generation:

Maintain adequate ventilation in the area.

#### Measures to protect the environment:

Avoid spreading product and keep it from spilling. Precautions or coming in contact with the ground, waterways, drains and vents.

#### Advice on general occupational hygiene:

Follow the general hygiene rules.

Precautions of use :

**Avoid any direct contact with the product.**

### **7.2. Conditions for safe storage, including any incompatibilities**

Storage conditions: Store in its original packaging in a cool dry place, away from light.

Technical measures: Close the container after use.

In case of transferring, reproduce the labelling.

Packaging materials: Preserve only in the container of origin.

Respect the general rules of incompatibility.

Storage :

**Store at 25°C max. in tightly sealed original container. Avoid prolonged exposure to light, heat and air.**

Storage areas and packaging conditions :

**Close carefully any already opened recipient and store it vertically to avoid any flow**

Protection against the fire and the explosion :

**Non-flammable**

### **7.3. Specific end use(s)**

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Wash the hands and any other zone exposed with soap and water before eating, drinking, to smoke and before leaving work.

## 8. SECTION 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

### 8.1. Control parameters

**Measures of technical order** : Avoid contact with eyes, skin and clothes. Do not ingest. Do not inhale vapors. Use proper personal protective equipment.

**Monitoring procedures** : If the product contains ingredients presenting exposure limits, it can turn out necessary to make an examination followed by the persons, by the atmosphere in the workplace either bodies living to end the efficiency of the ventilation or the other control measures or estimate the need to use of the material of protection of respiratory tracts. It is important to put back you in the European standard EN 689 concerning the methods to estimate the exhibition by inhalation to the chemical agents and to the national general documents of politics relative to the methods to determine dangerous substances.

PNEC Fresh water : **No data**

PNEC Fresh water sediment : **No data**

PNEC Marine water : **No data**

PNEC Marine sediment : **No data**

PNEC Soil : **No data**

VLEP short term mg/m<sup>3</sup> (98/24/CE) : **No data**

VLEP (8h) mg/m<sup>3</sup> (98/24/CE) : **No data**

DNEL - Inhalation : **No data**

DNEL - Skin contact : **No data**

### 8.2. Exposure controls

#### Appropriate technical controls :

No special ventilation requirements. Good general ventilation should be sufficient to control worker exposure to airborne contaminants. If this product contains ingredients with exposure limits, use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure.

#### Personal protection measures :

##### **Personal protection** :

-Protection des mains : Protection non requise.-Protection des yeux : Protection non requise.

-Protection respiratoire : En cas de ventilation insuffisante, porter un appareil respiratoire approprié.

**Respiratory protection** : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates that is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Filter apparatus (dust masks or half masks)

##### Type of filters

Type AX (Brown) : Organic compounds boiling point < 65°C

Type A (Brown) : Organic compounds boiling point > 65°C

Type B (Grey) : Inorganic gasses and fumes.

Type P (White) : Particles, dusts and aerosols

**Hand protection** : Impermeable and chemical resistant gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary >8 hours before piercing : vinyle disposable.

**Remark** : Recommended impermeable goggles do not only depend of his matter. Other factors can have a significant effect on

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impermeability, like their thickness or specific use or temperature conditions. In all cases, matter certificates should be selected. Ask your supply if the goggles are appropriate to this use.

**Eyes protection** : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Recommended : Splash goggles, safety glasses with side-shields.

**Skin protection** : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Body : Recommended : lab coat (sarrau), general.

Type 3 : Liquid impermeability

Type 4 : Aerosol impermeability

Type 6 : Impermeability limited to liquid splashes

Foot : Recommended : neoprene

Upper and sole resistant and impermeable (Hydrocarbure resistant).

## 9. SECTION 9 - PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

Appearance :	<b>Liquid</b>
Color :	<b>Colorless to pale yellow</b>
Odour :	<b>Woody, iris, floral, light</b>
Density at 20°C :	<b>[0.930 ; 0.934]</b>
Refractive index @ 20°C :	<b>[1.498 ; 1.502]</b>
Acid Value :	-
Melting point (°C) :	<b>&lt;-50°C</b>
Boiling point (°C) :	<b>270</b>
Flash point (°C) (close cup) :	<b>80.5</b>
Ignition temperature :	-
Explosive properties :	-
Impurities >0.01% :	-
Vapor pressure :	<b>0.003 mmHg @ 25°C</b>
Partition coefficient n-octanol/water :	<b>LogPow 4.6</b>
Peak #2 (%) :	<b>[Isomer iso-beta : 2.0 ; 6.0]</b>
Peak #3 (%) :	<b>[Isomer iso-alpha : 90.0 ; 95.00]</b>
Peak #1 (%) :	<b>[Isomer n-alpha : 0 ; 4.0]</b>
Relative density @ 25°C :	<b>[0.927 ; 0.931]</b>
Densité à 20/4°C :	<b>[0.928 ; 0.932]</b>
Refractive index at 25°C :	<b>[1.496 ; 1.500]</b>

### 9.2. Other information

Water solubility :	<b>No</b>
Solubility in alcohol (°) :	<b>Yes</b>

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## 10. SECTION 10 - STABILITY AND REACTIVITY

### 10.1. Reactivity

Avoid powerful oxidizing agents

### 10.2. Chemical stability

Stable under normal conditions.

Shelf life : **24 months, according to storage conditions**

### 10.3. Possibility of hazardous reactions

No hazardous reactions when stored and handled according to instructions.

### 10.4. Conditions to avoid

Avoid any potential source of heat.

### 10.5. Incompatible materials

NO CONCERNED

### 10.6. Hazardous decomposition products

**Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.

**Dangerous decomposition products:** No dangerous decomposition products known.

## 11. SECTION 11 - TOXICOLOGICAL INFORMATION

### 11.1. Information on toxicological

Phototoxicity :	<b>UV-VIS absorption spectrum: negative</b>
Genotoxicity in vivo :	<b>Micronucleus (Mouse) test: negative</b>
Genotoxicity in vitro :	<b>Ames test : negative</b>
LD50 oral (rat) :	<b>&gt;5000 mg/kg</b>
LD50 Dermal (rabbit) :	<b>&gt;5000 mg/kg</b>
Respiratory or Skin sensitization :	<b>Sensitizing (Mouse)</b>
Skin irritation :	<b>Irritant (Rabbit)</b>
Serious eye damage/irritation :	<b>No data</b>
Eyes irritation :	<b>Irritant (Rabbit)</b>

## 12. SECTION 12 - ECOLOGICAL INFORMATION

### 12.1. Toxicity

Do not leave the product, even diluted or in great quantity, penetrate the ground water, water or the drains.

LC50 Ecotoxicity : **10,9 mg/l (96h, Oncorhynchus mykiss)**



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EC50 Ecology : **No data**

CE50 (Aquatic fauna) : **2,65 mg/L (48h, Daphnia magna)**

CE50 (Aquatic flora) : **7,47 mg/L (72h, Selenastrum capricornutum)**

No observable adverse effect level (NOAEL) : **30 mg/kg (Rat, oral, 90d)**

No observed effect level (NOEL) : **No data**

### 12.2. Persistence and degradability

Biodegradability : **Easily biodegradable, 71%**

### 12.3. Bioaccumulative potential

Bioaccumulation (LogPow) : **4.6**

### 12.4. Mobility in soil

PNEC sol : **No data**

### 12.5. Results of PBT and vPvB assessment

vPvB : **This substance is not considered as very persistent nor very bioaccumulative**

PBT : **This substance is not considered as persistent, neither bioaccumulable nor toxin**

### 12.6. Other adverse effects

No data

## 13. SECTION 13 - DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

**Product** : Does not have to be evacuated with the refuse. Not let it penetrate in the sewers.

**Not cleaned packing** : Evacuation according to local reglementation.

## 14. SECTION 14 - TRANSPORT INFORMATION

ADR:



IMDG:



IATA:

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## 14.1. UN number

ADR : 3082 ( Tunnel code (E) )  
IMDG:3082  
IATA :3082

## 14.2. UN proper shipping name

ADR : Environmentally hazardous substance, liquid, n.o.s.,(3-méthyl-4-(2,6,6-triméthyl-2-cyclohexène-1-yl)-3-butène-2-one, Methyl-ionone)  
IMDG:Environmentally hazardous substance, liquid, n.o.s.,(3-méthyl-4-(2,6,6-triméthyl-2-cyclohexène-1-yl)-3-butène-2-one, Methyl-ionone)  
IATA :Environmentally hazardous substance, liquid, n.o.s.,(3-méthyl-4-(2,6,6-triméthyl-2-cyclohexène-1-yl)-3-butène-2-one, Methyl-ionone)

## 14.3. Transport hazard class(es)

ADR : 9  
IMDG:9  
IATA :9

## 14.4. Packing group

ADR : III  
IMDG:III  
IATA :III

## 14.5. Environmental hazards

IMDG : NO CONCERNED

## 14.6. Special precautions for user

**Avoid any direct contact with the product.**

## 14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

(Except particular case)

### IBC Liquid substances

Metal (31A, 31B, 31N)

Plastic (31H1, 31H2)

### GRV Solid substances

Metal (11A, 11B, 21A, 21N)

Plastic (11H1, 11H2, 21H1, 21H2)

## 15. SECTION 15 - REGULATORY INFORMATION

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

WGK : **2-ID3514**

Custom tariff : **2914 23 00 00**

### 15.2. Chemical safety assessment

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Exposure assessment : -

### 16. SECTION 16 - OTHER INFORMATION

#### Full H sentences text in point 3 :

H315 Causes skin irritation.  
H317 May cause an allergic skin reaction.  
H319 Causes serious eye irritation.  
H320 Causes eye irritation  
H411 Toxic to aquatic life with long lasting effects.

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#### Key literature references and sources for data

Sources for data : Information from supplier  
Literature references : ECHA  
Literature references EU : Reg. 1272/2008

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Safety data sheet according to REG. 1272/2008/CE and its amendments

These indications are founded on the current state of our knowledge, but do not constitute a guarantee as for the properties of the product and do not give place to a contractual legal report.

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