



Safety Data Sheet

Printed : 05/06/2023

Revised : CLP V1-R-1-CLP from 05/06/2023

ALLYL IONONE

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

1.1. Product identifier

ALLYL IONONE

Item code : ALL-1

N° CAS : 79-78-7

N° CE : 201-225-9

N° index REACH An VI : /

N° REACH (partially) : 01-2120746535-50-xxxx

IUPAC Name : **1-(2,6,6-Trimethyl-2-cyclohexenyl)hepta-1,6-dien-3-one; cetone V; hexalon**

Chemical / REACH name : **1-(2,6,6-trimethyl-2-cyclohexen-1-yl)hepta-1,6-dien-3-one**

Molecular formula : **C16 H24 O**

Molecular weight : **232.37**

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 / Flavours**

1.3. Details of the supplier of the safety data sheet

Company : PCW
45 Boulevard Marcel PAGNOL
Parc Aromagrasse
06130 GRASSE - FRANCE
Tel: +33 (0)4 92 42 35 00
Fax : +33 (0)4 92 42 35 19
Web : www.pcwfrance.com
Email : info@pcwfrance.com

Technical manager : 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

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ORFILA : +33(1) 45 42 59 59

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. Sens. 1 Sensitisation skin 1

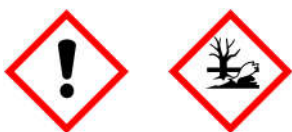
H317 - May cause an allergic skin reaction.

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. Sens. 1 Sensitisation skin 1

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.

P363 - Wash contaminated clothing before reuse.

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

2.3. Other hazards

The substance/mixture does not contain components considered to have endocrine disrupting properties according to Article 57(f) of REACH or Commission Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0,1 % or more.

Contains Allyl alpha-ionone, alpha-Tocopherol synthetic

PBT :

No data



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vPvB : **No data**

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

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

VOC (CARB) :

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

3. COMPOSITION / INFORMATION ON INGREDIENTS

List of reportable components:

3.1. Substances

Numéro d'identification	Substance	Classes danger & Phrases H	LCS / Facteurs M / ATE	Percent %
CAS# 79-78-7 EINECS# 201-225-9 REACH# /	Allyl alpha-ionone	Aquatic Chronic 2, Skin. Sens. 1B H411, H317		> 50 %
CAS# 1406-66-2 EINECS# - REACH# /	alpha-Tocopherol synthetic	Skin. Sens. 1B H317		[0-1]

The substance/mixture does not contain components considered to have endocrine disrupting properties according to Article 57(f) of REACH or Commission Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0,1 % or more.

3.2. Mixtures

Not concerned

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

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

Contact with skin: Wash immediately and abundantly with water and soap. Rinse then with clear water.

Contact with eyes: Abundant rinsing with water (15 minutes open eyelids) then washing with an ocular lotion standard Dacryoserum. In case of disorder, consult an ophtalmologist.

In case of ingestion: Do not induce vomiting, maintain the patient at rest. If problems persist, consult a doctor.

Soiled clothing: Withdraw soiled clothing and re-use them only after decontamination.

5. FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable extinguishing media: Use an extinguishing agent suitable for the surrounding fire. CO₂, powder, foam, specific liquid. Do not inhale the fumes.

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.

Hazardous combustion products:

Release of poison gases: Monoxide de carbone (CO), Dioxyde de carbon (CO₂), Oxyde d'azotes (NO_x), Dioxyde de soufre (SO₂), Cyanures (CN)

Auto-ignition temperature (°C) : -

5.3. Advice for firefighters

Never use a direct water jet.

Special protective equipment for fire-fighters:

Firefighters should wear appropriate protective equipment and self-contained breathing apparatus with full face mask operating in active pressure mode.

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 of flame).

Avoid skin/eye contact. Do not inhal vapours.

For emergency responders

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

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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

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. 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.

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.

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Respect the general rules of incompatibility.

Storage :	Keep under Nitrogen, at cool temperature (max 18°C). Avoid prolonged exposure to light, humidity 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)

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

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 with exposure limits, it may be necessary to carry out a follow-up examination of people, the workplace atmosphere or living organisms to determine the effectiveness of ventilation or other control measures or to assess the need for respiratory protective equipment. It is important to refer to the European standard EN 689 on methods for assessing inhalation exposure to chemical agents and to national policy documents on methods for determining hazardous 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 ³ (98/24/CE) :	No data
VLEP (8h) mg/m ³ (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 equipment :

- Hand protection: Protection not required.- Eye protection: Protection not required.- Respiratory protection: In case of insufficient ventilation, wear suitable respiratory equipment.

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- Hand protection: Protection not required.- Eye protection: Protection not required.- Respiratory protection: In case of insufficient ventilation, wear suitable respiratory equipment.

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 : The waterproofness of the recommended gloves does not only depend on their material. Also other factors can have an influence on the waterproofness, such as their thickness or specific use or temperature conditions. In any case, material certificates should be selected. Ask your supplier whether the gloves are suitable for this purpose.

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. PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance :	Liquid
Color :	Pale yellow
Odour :	Conform to the commercial description.
Densité à 20/4°C :	[0.927 ; 0.935]
Refractive index @ 20°C :	[1.503 ; 1.507]
Acid Value :	-
Melting point (°C) :	-
Boiling point (°C) :	-
Flash point (°C) (close cup) :	94
Ignition temperature :	-
Explosive properties :	-
Somme of isomers (by G.C.) (%) :	90%
Impurities >0.01% :	-



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Vapor pressure : **0.000498 mmHg @ 25.00 °C (litt)**

Partition coefficient n-octanol/water : **LogPow 5.30**

Peak #1 (%) : **[Hexalon, alpha ; 72-85%]**

Peak #2 (%) : **[hexalon, beta ; 10-16%]**

Relative density @ 25°C : **[0.926 ; 0.934]**

Density at 20°C : **[0.929 ; 0.937]**

9.2. Other information

Water solubility : **No**

Solubility in alcohol (°) : **Yes**

10. STABILITY AND REACTIVITY

10.1. Reactivity

Avoid powerful oxidising 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

Incompatibility with other materials: Strong acids, alkalis, oxidizing agent

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. TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Phototoxicity : **No data**

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Genotoxicity in vivo :	No data
Genotoxicity in vitro :	No data
LD50 oral (rat) :	6300 mg/kg
LD50 Dermal (rabbit) :	>5000 mg/kg
Respiratory or Skin sensitization :	No data
Skin irritation :	No data
Serious eye damage/irritation :	No data
Eyes irritation :	Moderate irritation

11.2. Information on other hazards

The product does not contain substances identified as having endocrine disrupting properties (human health) in concentrations equal to or greater than 0.1% (m/m).

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 :	No data
EC50 Ecology :	No data
CE50 (Aquatic fauna) :	No data
CE50 (Aquatic flora) :	No data
No observable adverse effect level (NOAEL) :	No data
No observed effect level (NOEL) :	No data

12.2. Persistence and degradability

Biodegradability :	No data
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12.3. Bioaccumulative potential

Bioaccumulation (LogPow) :	5.30 (litt)
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12.4. Mobility in soil

PNEC soil : No data

12.5. Results of PBT and vPvB assessment

vPvB	: No data
PBT	: No data

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12.6. Endocrine disrupting properties

The product does not contain substances identified as having endocrine disrupting properties (environment) in concentrations equal to or greater than 0.1% (m/m).

12.7. Other adverse effects

Not concerned

13. DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Product: Recommendation: Does not have to be evacuated with the refuse. Do not let penetrate into drains/waste water system.

Not cleaned packing: Recommendation: Evacuation in accordance with the regulations.

14. TRANSPORT INFORMATION

ADR/ADN/RID:



IMDG:



IATA:



14.1. UN number or ID number

ADR/ADN/RID : 3082 (Tunnel code (E))

IMDG:3082

IATA :3082

14.2. UN proper shipping name

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ADR/ADN/RID : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.(Reaction mass of 1-(2,6,6-trimethylcyclohex-2-en-1-yl)hepta-1,6-dien-3-one and 1-(2,6,6-trimethylcyclohex-1-en-1-yl)hepta-1,6-dien-3-one)

IMDG:ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.(Reaction mass of 1-(2,6,6-trimethylcyclohex-2-en-1-yl)hepta-1,6-dien-3-one and 1-(2,6,6-trimethylcyclohex-1-en-1-yl)hepta-1,6-dien-3-one)

IATA :ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.(Reaction mass of 1-(2,6,6-trimethylcyclohex-2-en-1-yl)hepta-1,6-dien-3-one and 1-(2,6,6-trimethylcyclohex-1-en-1-yl)hepta-1,6-dien-3-one)

14.3. Transport hazard class(es)

ADR/ADN/RID : 9

IMDG:9

IATA :9

14.4. Packing group

ADR/ADN/RID : III

IMDG:III

IATA :III

14.5. Environmental hazards

IMDG :

14.6. Special precautions for user

Precautions of use : **Avoid any direct contact with the product.**

14.7. Maritime transport in bulk according to IMO instruments

(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. REGULATORY INFORMATION

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

WGK : **2-ID5785**

Custom tariff : **2914 23 00 00**

15.2. Chemical safety assessment

Exposure assessment : -

16. OTHER INFORMATION



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Full H sentences text in point 3 :

H317 May cause an allergic skin reaction.

H411 Toxic to aquatic life with long lasting effects.

Material security data sheet according to 2020/878/CEE.

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.