



alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878
Issue date: 4/24/2024 Revision date: 1/29/2026 Supersedes version of: 4/24/2024 Version: 2.0

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

| | |
|------------------------|--|
| Product form | : Substance |
| Substance name | : alpha-Irone |
| IUPAC name | : 4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one |
| EC-No. | : 201-219-6 |
| CAS-No. | : 79-69-6 |
| REACH registration No. | : 01-2120734727-47 |
| Product code | : 23091 |
| Formula | : C ₁₄ H ₂₂ O |
| Product group | : Trade product |

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

Relevant identified uses

| | |
|------------------------------|----------------------------------|
| Intended for general public | |
| Main use category | : Professional use, Consumer use |
| Use of the substance/mixture | : Fragrance raw material |

1.3. Details of the supplier of the safety data sheet

De Hekserij
Sporstraat 57
8271 RG IJsselmuiden
Nederland
T +31 383 557 927
hekserij@hekserij.nl, www.hekserij.nl

1.4. Emergency telephone number

No additional information available

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Hazardous to the aquatic environment – Chronic Hazard, H411
Category 2
Full text of H- and EUH-statements: see section 16

Adverse physicochemical, human health and environmental effects

Toxic to aquatic life with long lasting effects.

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



GHS09

Signal word (CLP)

: -

Hazard statements (CLP)

: H411 - Toxic to aquatic life with long lasting effects.

Precautionary statements (CLP)

: P102 - Keep out of reach of children.
P273 - Avoid release to the environment.
P391 - Collect spillage.

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

P501 - Dispose of contents and container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

2.3. Other hazards

Contains no PBT and/or vPvB substances $\geq 0.1\%$ assessed in accordance with REACH Annex XIII

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Multi-constituent
Name : alpha-Irone
CAS-No. : 79-69-6
EC-No. : 201-219-6

| Name | Product identifier | % | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
|--|---|-----------|---|
| 4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one | CAS-No.: 79-69-6 EC-No.: 201-219-6 REACH-no: 01-2120734727-47 | ≥ 50 | Aquatic Chronic 2, H411 |

Full text of H- and EUH-statements: see section 16

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : If you feel unwell, seek medical advice.
First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.
First-aid measures after skin contact : Wash skin with plenty of water.
First-aid measures after eye contact : Rinse eyes with water as a precaution.
First-aid measures after ingestion : Call a poison center or a doctor if you feel unwell.
Self protection of the first-aiders : First aid workers will be equipped with suitable personal protective equipment.

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

Symptoms/effects after inhalation : None under normal conditions.
Symptoms/effects after skin contact : None under normal conditions.
Symptoms/effects after eye contact : None under normal conditions.
Symptoms/effects after ingestion : None under normal conditions.

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 : Water spray. Dry powder. Foam. Carbon dioxide.
Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

Fire hazard : No fire hazard.
Explosion hazard : No direct explosion hazard.
Hazardous decomposition products in case of fire : Toxic fumes may be released.

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

5.3. Advice for firefighters

- | | |
|--------------------------------|---|
| Firefighting instructions | : Fight fire from safe distance and protected location. Do not enter fire area without proper protective equipment, including respiratory protection. |
| Protection during firefighting | : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing. |

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- | | |
|------------------|--|
| General measures | : Stop leak if safe to do so. Notify authorities if product enters sewers or public waters. Absorb spillage to prevent material damage. |
|------------------|--|

For non-emergency personnel

- | | |
|----------------------|---|
| Protective equipment | : Wear recommended personal protective equipment. |
| Emergency procedures | : Ventilate spillage area. |

For emergency responders

- | | |
|----------------------|---|
| Protective equipment | : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection". |
| Emergency procedures | : Evacuate unnecessary personnel. Stop leak if safe to do so. |

6.2. Environmental precautions

Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

- | | |
|-------------------------|---|
| For containment | : Collect spillage. Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams. Stop leak without risks if possible. |
| Methods for cleaning up | : Take up liquid spill into absorbent material. |
| Other information | : Dispose of materials or solid residues at an authorized site. |

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

- | | |
|-----------------------------------|---|
| Additional hazards when processed | : Not expected to present a significant hazard under anticipated conditions of normal use. |
| Precautions for safe handling | : Ensure good ventilation of the work station. Wear personal protective equipment. |
| Hygiene measures | : Do not eat, drink or smoke when using this product. Always wash hands after handling the product. |

7.2. Conditions for safe storage, including any incompatibilities

- | | |
|---------------------|---|
| Technical measures | : Keep in a cool, well-ventilated place away from heat. |
| Storage conditions | : Keep cool. Protect from sunlight. |
| Packaging materials | : Store always product in container of same material as original container. |

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

8.2. Exposure controls

Appropriate engineering controls

Appropriate engineering controls:

Ensure good ventilation of the work station.

Personal protection equipment

Personal protective equipment:

Wear recommended personal protective equipment.

Personal protective equipment symbol(s):



Eye and face protection

Eye protection:

Safety glasses

Skin protection

Skin and body protection:

Wear suitable protective clothing

Hand protection:

Protective gloves

Respiratory protection

Respiratory protection:

In case of insufficient ventilation, wear suitable respiratory equipment

Environmental exposure controls

Environmental exposure controls:

Avoid release to the environment.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|---|--|
| Physical state | : Liquid |
| Colour | : colourless to pale yellow. |
| Odour | : Not available |
| Odour threshold | : Not available |
| Melting point | : < -50 °C |
| Freezing point | : Not available |
| Boiling point | : 290.85 °C Atm. press.: 101,325 kPa |
| Flammability | : Non flammable. |
| Lower explosion limit | : Not available |
| Upper explosion limit | : Not available |
| Flash point | : 127 °C Atm. press.: 101325 Pa |
| Auto-ignition temperature | : Not available |
| Decomposition temperature | : Not available |
| pH | : Not available |
| Viscosity, kinematic | : Not available |
| Solubility | : Insoluble in water. |
| Partition coefficient n-octanol/water (Log Kow) | : Not available |
| Partition coefficient n-octanol/water (Log Pow) | : 4 |
| Vapour pressure | : 0.4 Pa Temp.: 20 °C |
| Vapour pressure at 50°C | : Not available |
| Density | : 0.934 g/cm³ Type: 'density' Temp.: 20 °C |
| Relative density | : 0.928 – 0.936 |
| Relative vapour density at 20°C | : Not available |
| Particle characteristics | : Not applicable |

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

10.2. Chemical stability

Stable under normal conditions.

10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

SECTION 11: Toxicological information

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

| | |
|-----------------------------|------------------|
| Acute toxicity (oral) | : Not classified |
| Acute toxicity (dermal) | : Not classified |
| Acute toxicity (inhalation) | : Not classified |

4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one (79-69-6)

| | |
|---------------|--|
| LD50 oral rat | 5000 mg/kg bodyweight Animal: rat, Guideline: other: |
|---------------|--|

| | |
|-----------------------------------|------------------|
| Skin corrosion/irritation | : Not classified |
| Serious eye damage/irritation | : Not classified |
| Respiratory or skin sensitisation | : Not classified |
| Germ cell mutagenicity | : Not classified |
| Carcinogenicity | : Not classified |
| Reproductive toxicity | : Not classified |
| STOT-single exposure | : Not classified |
| STOT-repeated exposure | : Not classified |
| Aspiration hazard | : Not classified |

11.2. Information on other hazards

No additional information available

SECTION 12: Ecological information

12.1. Toxicity

| | |
|---|--|
| Ecology - general | : Toxic to aquatic life with long lasting effects. |
| Hazardous to the aquatic environment, short-term (acute) | : Not classified |
| Hazardous to the aquatic environment, long-term (chronic) | : Toxic to aquatic life with long lasting effects. |

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one (79-69-6)

| | |
|----------------------|---|
| EC50 - Crustacea [1] | 3.7 mg/l Test organisms (species): Daphnia magna |
| EC50 72h - Algae [1] | > 5.1 mg/l Test organisms (species): Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) |
| EC50 72h - Algae [2] | 4.4 mg/l Test organisms (species): Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) |

12.2. Persistence and degradability

alpha-Irone (79-69-6)

| | |
|-------------------------------|------------------------|
| Persistence and degradability | Not rapidly degradable |
|-------------------------------|------------------------|

4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one (79-69-6)

| | |
|-------------------------------|------------------------|
| Persistence and degradability | Not rapidly degradable |
|-------------------------------|------------------------|

12.3. Bioaccumulative potential

alpha-Irone (79-69-6)

| | |
|---|---|
| Partition coefficient n-octanol/water (Log Pow) | 4 |
|---|---|

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Endocrine disrupting properties

No additional information available

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

| | |
|--|---|
| Regional waste regulation | : Disposal must be done according to official regulations. |
| Waste treatment methods | : Dispose of contents/container in accordance with licensed collector's sorting instructions. |
| Sewage disposal recommendations | : Disposal must be done according to official regulations. |
| Product/Packaging disposal recommendations | : Disposal must be done according to official regulations. |
| Additional information | : Do not re-use empty containers. |

SECTION 14: Transport information






In accordance with ADR / IMDG / IATA / ADN / RID

| ADR | IMDG | IATA | ADN | RID |
|-------------------------------------|---------|---------|---------|---------|
| 14.1. UN number or ID number | | | | |
| UN 3082 | UN 3082 | UN 3082 | UN 3082 | UN 3082 |

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

| ADR | IMDG | IATA | ADN | RID |
|--|---|---|--|---|
| 14.2. UN proper shipping name | | | | |
| ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone) | ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone) | Environmentally hazardous substance, liquid, n.o.s. (alpha-Irone) | ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone) | ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone) |
| Transport document description | | | | |
| UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone), 9, III, (-) | UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone), 9, III, MARINE POLLUTANT | UN 3082 Environmentally hazardous substance, liquid, n.o.s. (alpha-Irone), 9, III | UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone), 9, III | UN 3082 ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (alpha-Irone), 9, III |
| 14.3. Transport hazard class(es) | | | | |
| 9 | 9 | 9 | 9 | 9 |
|  |  |  |  |  |
| 14.4. Packing group | | | | |
| III | III | III | III | III |
| 14.5. Environmental hazards | | | | |
| Dangerous for the environment: Yes | Dangerous for the environment: Yes Marine pollutant: Yes EmS-No. (Fire): F-A EmS-No. (Spillage): S-F | Dangerous for the environment: Yes | Dangerous for the environment: Yes | Dangerous for the environment: Yes |
| No supplementary information available | | | | |

14.6. Special precautions for user

Overland transport

Classification code (ADR) : M6
Special provisions (ADR) : 274, 335, 375, 601, 650
Limited quantities (ADR) : 5I
Excepted quantities (ADR) : E1
Packing instructions (ADR) : P001, IBC03, LP01, R001
Special packing provisions (ADR) : PP1
Mixed packing provisions (ADR) : MP19
Portable tank and bulk container instructions (ADR) : T4
Portable tank and bulk container special provisions (ADR) : TP1, TP29
Tank code (ADR) : LGBV
Vehicle for tank carriage : AT
Transport category (ADR) : 3
Special provisions for carriage - Packages (ADR) : V12
Special provisions for carriage - Loading, unloading and handling (ADR) : CV13
Hazard identification number (Kemler No.) : 90
Orange plates :



Tunnel restriction code (ADR) : -

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

Transport by sea

| | |
|-----------------------------------|----------------------|
| Special provisions (IMDG) | : 274, 335, 375, 969 |
| Limited quantities (IMDG) | : 5 L |
| Excepted quantities (IMDG) | : E1 |
| Packing instructions (IMDG) | : LP01, P001 |
| Special packing provisions (IMDG) | : PP1 |
| IBC packing instructions (IMDG) | : IBC03 |
| Tank instructions (IMDG) | : T4 |
| Tank special provisions (IMDG) | : TP1, TP29 |
| Stowage category (IMDG) | : A |

Air transport

| | |
|--|-------------------------|
| PCA Excepted quantities (IATA) | : E1 |
| PCA Limited quantities (IATA) | : Y964 |
| PCA limited quantity max net quantity (IATA) | : 30kgG |
| PCA packing instructions (IATA) | : 964 |
| PCA max net quantity (IATA) | : 450L |
| CAO packing instructions (IATA) | : 964 |
| CAO max net quantity (IATA) | : 450L |
| Special provisions (IATA) | : A97, A158, A197, A215 |
| ERG code (IATA) | : 9L |

Inland waterway transport

| | |
|-----------------------------------|---------------------------|
| Classification code (ADN) | : M6 |
| Special provisions (ADN) | : 274, 335, 375, 601, 650 |
| Limited quantities (ADN) | : 5 L |
| Excepted quantities (ADN) | : E1 |
| Carriage permitted (ADN) | : T |
| Equipment required (ADN) | : PP |
| Number of blue cones/lights (ADN) | : 0 |

Rail transport

| | |
|---|---------------------------|
| Classification code (RID) | : M6 |
| Special provisions (RID) | : 274, 335, 375, 601, 650 |
| Limited quantities (RID) | : 5L |
| Excepted quantities (RID) | : E1 |
| Packing instructions (RID) | : P001, IBC03, LP01, R001 |
| Special packing provisions (RID) | : PP1 |
| Mixed packing provisions (RID) | : MP19 |
| Portable tank and bulk container instructions (RID) | : T4 |
| Portable tank and bulk container special provisions (RID) | : TP1, TP29 |
| Tank codes for RID tanks (RID) | : LGBV |
| Transport category (RID) | : 3 |
| Special provisions for carriage – Packages (RID) | : W12 |
| Special provisions for carriage - Loading, unloading and handling (RID) | : CW13, CW31 |
| Colis express (express parcels) (RID) | : CE8 |
| Hazard identification number (RID) | : 90 |

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

SECTION 15: Regulatory information

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

EU-Regulations

REACH Annex XVII (Restriction List)

EU restriction list (REACH Annex XVII)

| Reference code | Applicable on | Entry title or description |
|----------------|--|---|
| 3(c) | alpha-Irone ; 4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one | Substances or mixtures fulfilling the criteria for any of the following hazard classes or categories set out in Annex I to Regulation (EC) No 1272/2008: Hazard class 4.1 |

REACH Annex XIV (Authorisation List)

Not listed on REACH Annex XIV (Authorisation List)

REACH Candidate List (SVHC)

Contains no substance(s) listed on the REACH Candidate List

PIC Regulation (Prior Informed Consent)

Contains no substance(s) listed on the PIC list (Regulation EU 649/2012 concerning the export and import of hazardous chemicals)

POP Regulation (Persistent Organic Pollutants)

Contains no substance(s) listed on the POP list (Regulation EU 2019/1021 on persistent organic pollutants)

Ozone Regulation (2024/590)

Not listed on the Ozone Depletion list (Regulation EU 2024/590)

Council Regulation (EC) for the control of dual-use items

Contains no substance subject to the COUNCIL REGULATION (EC) for the control of dual-use items

Explosives Precursors Regulation (EU 2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors)

Drug Precursors Regulation (EC 273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances)

National regulations

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed
SZW-lijst van mutagene stoffen : The substance is not listed
SZW-lijst van reprotoxische stoffen – Borstvoeding : The substance is not listed
SZW-lijst van reprotoxische stoffen – Vruchtbaarheid : The substance is not listed
SZW-lijst van reprotoxische stoffen – Ontwikkeling : The substance is not listed

15.2. Chemical safety assessment

No chemical safety assessment has been carried out

SECTION 16: Other information

Abbreviations and acronyms:

| | |
|-------|---|
| ACGIH | American Conference of Government Industrial Hygienists |
| ADN | European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways |
| ADR | European Agreement concerning the International Carriage of Dangerous Goods by Road |
| ATE | Acute Toxicity Estimate |

| Abbreviations and acronyms: | |
|-----------------------------|--|
| BCF | Bioconcentration factor |
| BLV | Biological limit value |
| BOD | Biochemical oxygen demand (BOD) |
| CAS-No. | Chemical Abstract Service number |
| CLP | Classification Labelling Packaging Regulation; Regulation (EC) No 1272/2008 |
| COD | Chemical oxygen demand (COD) |
| CSA | Chemical safety assessment |
| DMEL | Derived Minimal Effect level |
| DNEL | Derived-No Effect Level |
| EC-No. | European Community number |
| EC50 | Median effective concentration |
| ED | Endocrine disruptor |
| EN | European Standard |
| EWC | European waste catalogue |
| IARC | International Agency for Research on Cancer |
| IATA | International Air Transport Association |
| IMDG | International Maritime Dangerous Goods |
| LC50 | Median lethal concentration |
| LD50 | Median lethal dose |
| LOAEL | Lowest Observed Adverse Effect Level |
| Log Kow | Partition coefficient n-octanol/water (Log Kow) |
| Log Pow | Partition coefficient n-octanol/water (Log Pow) |
| MAK | maximum workplace concentration |
| NOAEC | No-Observed Adverse Effect Concentration |
| NOAEL | No-Observed Adverse Effect Level |
| NOEC | No-Observed Effect Concentration |
| N.O.S. | Not Otherwise Specified |
| OECD | Organisation for Economic Co-operation and Development |
| OEL | Occupational Exposure Limit |
| OSHA | Occupational Safety Health Administration |
| PBT | Persistent Bioaccumulative Toxic |
| PNEC | Predicted No-Effect Concentration |
| PPE | Personal protection equipment |
| RID | Regulations concerning the International Carriage of Dangerous Goods by Rail |
| SDS | Safety Data Sheet |
| STP | Sewage treatment plant |
| TF | Technical function |
| ThOD | Theoretical oxygen demand (ThOD) |
| TLM | Median Tolerance Limit |

alpha-Irone

Safety Data Sheet

according to the REACH Regulation (EC) 1907/2006 amended by Regulation (EU) 2020/878

Abbreviations and acronyms:

| | |
|------|--|
| TWA | Time Weighted Average |
| VOC | Volatile Organic Compounds |
| vPvB | Very Persistent and Very Bioaccumulative |
| UFI | Unique Formula Identifier |

Full text of H- and EUH-statements:

| | |
|-------------------|---|
| Aquatic Chronic 2 | Hazardous to the aquatic environment – Chronic Hazard, Category 2 |
| H411 | Toxic to aquatic life with long lasting effects. |

Safety Data Sheet (SDS), EU

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.