



DE HEKSERIJ

# 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	:	C14H22O
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  
Spoorstraat 57  
8271 RG IJsselmuiden  
Nederland  
T +31 383 557 927  
[hekserij@hekserij.nl](mailto:hekserij@hekserij.nl), [www.hekserij.nl](http://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 ≥ 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-aider : 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.

### 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

### 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

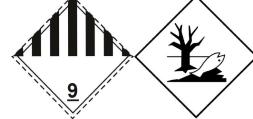
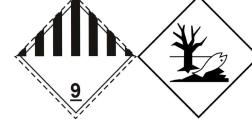
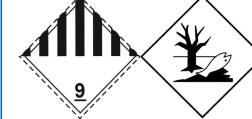
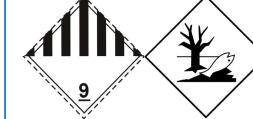
In accordance with ADR / IMDG / IATA / ADN / RID

ADR	IMDG	IATA	ADN	RID
<b>14.1. UN number or ID number</b>				
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
<b>14.2. UN proper shipping name</b>				
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)
<b>Transport document description</b>				
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
<b>14.3. Transport hazard class(es)</b>				
9	9	9	9	9
				
<b>14.4. Packing group</b>				
III	III	III	III	III
<b>14.5. Environmental hazards</b>				
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				
<b>14.6. Special precautions for user</b>				
<b>Overland transport</b>				
Classification code (ADR)	: M6			
Special provisions (ADR)	: 274, 335, 375, 601, 650			
Limited quantities (ADR)	: 5l			
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 –	: The substance is not listed
Vruchtbareheid	
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

# alpha-Irone

## Safety Data Sheet

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

<b>Abbreviations and acronyms:</b>	
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.