

Safety data sheet
according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025





Version number 1

Revision: 08.01.2025

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

- **1.1 Product identifier**
- **Trade name:** 2-Octanone natural
- **Product number:** 1221
- **CAS Number:**
111-13-7
- **EC number:**
203-837-1
- **1.2 Relevant identified uses of the substance or mixture and uses advised against**
No further relevant information available.
- **Application of the substance / the mixture** Flavoring Ingredients
- **1.3 Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Advanced Biotech
10 Taft Road
Totowa, NJ 07512 USA
- **Further information obtainable from:**
Product Safety Department
productsafety@adv-bio.com
- **1.4 Emergency telephone number:**
Infotrac: 1-800-535-5053 (Domestic) & 1-352-323-3500 (International)
Email: responders@infotrac.net & During normal business hours: 1-973-339-6242

SECTION 2: Hazards identification

- **2.1 Classification of the substance or mixture**
- **Classification according to Regulation (EC) No 1272/2008**
-  GHS02 flame
Flam. Liq. 3 H226 Flammable liquid and vapour.
-  GHS07
Acute Tox. 4 H302 Harmful if swallowed.
Skin Irrit. 2 H315 Causes skin irritation.
Eye Irrit. 2 H319 Causes serious eye irritation.
- **Labelling according to Regulation (EC) No 1272/2008**
The substance is classified and labelled according to the CLP regulation.
- **Hazard pictograms**
-  
GHS02 GHS07
- **Signal word** Warning

(Contd. on page 2)

Safety data sheet
according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 1)

· **Hazard-determining components of labelling:**

2-Octanone

· **Hazard statements**

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

· **Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P241 Use explosion-proof [electrical/ventilating/lighting] equipment.

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

· **2.3 Other hazards**

· **Results of PBT and vPvB assessment**

· **PBT:** Not applicable.

· **vPvB:** Not applicable.

SECTION 3: Composition/information on ingredients

· **3.1 Substances**

· **CAS No. Description**

CAS: 111-13-7 2-Octanone

· **Identification number(s)**

· **EC number:** 203-837-1

· **Acute toxicity estimate (ATE) values** LD50 oral: 500 mg/kg

SECTION 4: First aid measures

· **4.1 Description of first aid measures**

· **General information:**

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

· **After inhalation:** Supply fresh air; consult doctor in case of complaints.

· **After skin contact:** Immediately rinse with water.

· **After eye contact:**

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

· **After swallowing:** Call for a doctor immediately.

· **4.2 Most important symptoms and effects, both acute and delayed**

No further relevant information available.

· **4.3 Indication of any immediate medical attention and special treatment needed**

No further relevant information available.

(Contd. on page 3)

Safety data sheet

according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 2)

SECTION 5: Firefighting measures

- **5.1 Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet
- **5.2 Special hazards arising from the substance or mixture** No further relevant information available.
- **5.3 Advice for firefighters**
- **Protective equipment:** No special measures required.
- **Additional information**
Cool endangered receptacles with water spray.
Collect contaminated fire fighting water separately. It must not enter the sewage system.

SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures**
Wear protective equipment. Keep unprotected persons away.
- **6.2 Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **6.3 Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
- **6.4 Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

SECTION 7: Handling and storage

- **7.1 Precautions for safe handling** No special precautions are necessary if used correctly.
- **Information about fire - and explosion protection:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
- **7.2 Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:**
Please refer to the product specification and/or Certificate of Analysis for product storage requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** Keep container tightly sealed.
- **7.3 Specific end use(s)** No further relevant information available.

SECTION 8: Exposure controls/personal protection

- **8.1 Control parameters**
- **Ingredients with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists valid during the making were used as a basis.
- **8.2 Exposure controls**
- **Appropriate engineering controls** No further data; see section 7.

(Contd. on page 4)

Safety data sheet
according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 3)

- **Individual protection measures, such as personal protective equipment**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing
Wash hands before breaks and at the end of work.
Avoid contact with the eyes.
Avoid contact with the eyes and skin.
- **Respiratory protection:** Not required.
- **Hand protection**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material should be based on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

- **Penetration time of glove material**

The exact break through time has to be determined by the manufacturer of the protective gloves and has to be observed.

- **Eye/face protection**



Tightly sealed goggles

SECTION 9: Physical and chemical properties

- **9.1 Information on basic physical and chemical properties**

- | | |
|---|------------------------------------|
| · General Information | Molecular Weight: 128.21 g/mol |
| · Physical state | Liquid |
| · Colour: | According to product specification |
| · Odour: | According to product specification |
| · Odour threshold: | Not determined. |
| · Melting point/freezing point: | -16 °C |
| · Boiling point or initial boiling point and boiling range | 173.5 °C |
| · Flammability | Flammable. |
| · Lower and upper explosion limit | |
| · Lower: | Not determined. |
| · Upper: | Not determined. |
| · Flash point: | 52 °C |
| · Auto-ignition temperature: | 420 °C |
| · Decomposition temperature: | Not determined. |
| · pH | Not determined. |

(Contd. on page 5)

Safety data sheet
 according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 4)

· Viscosity:	
· Kinematic viscosity	Not determined.
· Dynamic:	Not determined.
· Solubility	
· water:	Not miscible or difficult to mix.
· Partition coefficient n-octanol/water (log value)	Not determined.
· Vapour pressure at 20 °C:	1 hPa
· Density and/or relative density	
· Density at 20 °C:	0.82 g/cm ³
· Relative density	Not determined.
· Refractive Index	
· Vapour density	Not determined.

· 9.2 Other information	
· Appearance:	
· Form:	Liquid
· Important information on protection of health and environment, and on safety.	
· Ignition temperature:	Not determined.
· Explosive properties:	Not determined.
· Solvent content:	
· VOC (EC)	0.00 %
· Change in condition	
· Evaporation rate	Not determined.

· Information with regard to physical hazard classes	
· Explosives	Void
· Flammable gases	Void
· Aerosols	Void
· Oxidising gases	Void
· Gases under pressure	Void
· Flammable liquids	Flammable liquid and vapour.
· Flammable solids	Void
· Self-reactive substances and mixtures	Void
· Pyrophoric liquids	Void
· Pyrophoric solids	Void
· Self-heating substances and mixtures	Void
· Substances and mixtures, which emit flammable gases in contact with water	Void
· Oxidising liquids	Void
· Oxidising solids	Void
· Organic peroxides	Void
· Corrosive to metals	Void
· Desensitised explosives	Void

SECTION 10: Stability and reactivity

- **10.1 Reactivity** No further relevant information available.

(Contd. on page 6)

Safety data sheet
according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 5)

- **10.2 Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
- **10.3 Possibility of hazardous reactions** No dangerous reactions known.
- **10.4 Conditions to avoid** No further relevant information available.
- **10.5 Incompatible materials:** No further relevant information available.
- **10.6 Hazardous decomposition products:** No dangerous decomposition products known.

SECTION 11: Toxicological information

- **11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008**
- **Acute toxicity** Harmful if swallowed.

- **LD/LC50 values relevant for classification:**

ATE (Acute Toxicity Estimates)

Oral	LD50	500 mg/kg (ATE)
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CAS: 111-13-7 2-Octanone

Oral	LD50	500 mg/kg (ATE)
		3,824 mg/kg (mouse)

- **Primary irritant effect:**
- **Skin corrosion/irritation** Causes skin irritation.
- **Serious eye damage/irritation** Causes serious eye irritation.
- **Respiratory or skin sensitisation** Based on available data, the classification criteria are not met.
- **Germ cell mutagenicity** Based on available data, the classification criteria are not met.
- **Carcinogenicity** Based on available data, the classification criteria are not met.
- **Reproductive toxicity** Based on available data, the classification criteria are not met.
- **STOT-single exposure** Based on available data, the classification criteria are not met.
- **STOT-repeated exposure** Based on available data, the classification criteria are not met.
- **Aspiration hazard** Based on available data, the classification criteria are not met.
- **11.2 Information on other hazards**

- **Endocrine disrupting properties**

Substance is not listed.

SECTION 12: Ecological information

- **12.1 Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **12.2 Persistence and degradability** No further relevant information available.
- **12.3 Bioaccumulative potential** No further relevant information available.
- **12.4 Mobility in soil** No further relevant information available.
- **12.5 Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **12.6 Endocrine disrupting properties**
The product does not contain substances with endocrine disrupting properties.

(Contd. on page 7)

Safety data sheet

according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural



(Contd. of page 6)

- **12.7 Other adverse effects**
- **Additional ecological information:**
- **General notes:**
Water hazard class 1 (German Regulation) (Assessment by list): slightly hazardous for water
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

SECTION 13: Disposal considerations

- **13.1 Waste treatment methods**
- **Recommendation**
Must not be disposed together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packaging:**
- **Recommendation:** Disposal must be made according to official regulations.

SECTION 14: Transport information

- | | |
|--|--|
| <ul style="list-style-type: none"> · 14.1 UN number or ID number · ADR, IMDG, IATA | <p style="text-align: right;">UN1224</p> |
| <ul style="list-style-type: none"> · 14.2 UN proper shipping name · ADR · IMDG, IATA | <p style="text-align: right;">1224 KETONES, LIQUID, N.O.S. (2-Octanone)
KETONES, LIQUID, N.O.S. (2-Octanone)</p> |
| <ul style="list-style-type: none"> · 14.3 Transport hazard class(es) · ADR <div style="text-align: center; margin: 10px 0;">  </div> <ul style="list-style-type: none"> · Class · Label | <p style="text-align: right;">3 (F1) Flammable liquids.
3</p> |
| <ul style="list-style-type: none"> · IMDG, IATA <div style="text-align: center; margin: 10px 0;">  </div> <ul style="list-style-type: none"> · Class · Label | <p style="text-align: right;">3 Flammable liquids.
3</p> |
| <ul style="list-style-type: none"> · 14.4 Packing group · ADR, IMDG, IATA | <p style="text-align: right;">III</p> |
| <ul style="list-style-type: none"> · 14.5 Environmental hazards: · Marine pollutant: | <p style="text-align: right;">No</p> |
| <ul style="list-style-type: none"> · 14.6 Special precautions for user · Hazard identification number (Kemler code): · EMS Number: | <p style="text-align: right;">Warning: Flammable liquids.
30
F-E,S-D</p> |

(Contd. on page 8)

Safety data sheet
 according to Regulation (EC) No 1907/2006, Article 31

Printing date 24.01.2025

Version number 1

Revision: 08.01.2025

Trade name: 2-Octanone natural

(Contd. of page 7)

· Stowage Category	A
· 14.7 Maritime transport in bulk according to IMO instruments	Not applicable.
· Transport/Additional information:	
· ADR	
· Limited quantities (LQ)	5L
· Excepted quantities (EQ)	Code: E1 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 1000 ml
· Transport category	3
· Tunnel restriction code	D/E
· IMDG	
· Limited quantities (LQ)	5L
· Excepted quantities (EQ)	Code: E1 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 1000 ml
· UN "Model Regulation":	UN 1224 KETONES, LIQUID, N.O.S. (2-OCTANONE), 3, III

SECTION 15: Regulatory information

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

· **Labelling according to Regulation (EC) No 1272/2008**

The substance is classified and labelled according to the CLP regulation.

· **Hazard pictograms**



GHS02 GHS07

· **Signal word** Warning

· **Hazard-determining components of labelling:**

2-Octanone

· **Hazard statements**

H226 Flammable liquid and vapour.

H302 Harmful if swallowed.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

· **Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P241 Use explosion-proof [electrical/ventilating/lighting] equipment.

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

(Contd. on page 9)

Safety data sheet
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Trade name: 2-Octanone natural

(Contd. of page 8)

P403+P235 Store in a well-ventilated place. Keep cool.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Directive 2012/18/EU**
- **Named dangerous substances - ANNEX I** Substance is not listed.
- **Seveso category** P5c FLAMMABLE LIQUIDS
- **Qualifying quantity (tonnes) for the application of lower-tier requirements** 5,000 t
- **Qualifying quantity (tonnes) for the application of upper-tier requirements** 50,000 t
- **REGULATION (EC) No 1907/2006 ANNEX XVII** Conditions of restriction: 3

· **DIRECTIVE 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment – Annex II**

Substance is not listed.

· **REGULATION (EU) 2019/1148**

· **Annex I - RESTRICTED EXPLOSIVES PRECURSORS (Upper limit value for the purpose of licensing under Article 5(3))**

Substance is not listed.

· **Annex II - REPORTABLE EXPLOSIVES PRECURSORS**

Substance is not listed.

· **Regulation (EC) No 273/2004 on drug precursors**

Substance is not listed.

· **Regulation (EC) No 111/2005 laying down rules for the monitoring of trade between the Community and third countries in drug precursors**

Substance is not listed.

· **15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· **Department issuing SDS:** Product safety department

· **Contact:**

Product Safety Department
productsafety@adv-bio.com

· **Abbreviations and acronyms:**

ADR: Accord relatif au transport international des marchandises dangereuses par route (European Agreement Concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonised System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

vPvB: very Persistent and very Bioaccumulative

ATE: Acute toxicity estimate values

Flam. Liq. 3: Flammable liquids – Category 3

Acute Tox. 4: Acute toxicity – Category 4

Skin Irrit. 2: Skin corrosion/irritation – Category 2

Eye Irrit. 2: Serious eye damage/eye irritation – Category 2