

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 16.01.2024




Version number 1

Revision: 16.01.2024

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

- **1.1 Product identifier**
- **Trade name:** Isovaleraldehyde natural
- **Product number:** 1185
- **CAS Number:**  
590-86-3
- **EC number:**  
209-691-5
- **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. 2      H225 Highly flammable liquid and vapour.
-  GHS09 environment  
 Aquatic Chronic 2    H411 Toxic to aquatic life with long lasting effects.
-  GHS07  
 Eye Irrit. 2      H319 Causes serious eye irritation.  
 Skin Sens. 1B    H317 May cause an allergic skin reaction.  
 STOT SE 3      H335 May cause respiratory irritation.
- **Labelling according to Regulation (EC) No 1272/2008**  
The substance is classified and labelled according to the GB CLP regulation.

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· **Hazard pictograms**



GHS02 GHS07 GHS09

· **Signal word** Danger

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

3-Methylbutyraldehyde

· **Hazard statements**

H225 Highly flammable liquid and vapour.

H319 Causes serious eye irritation.

H317 May cause an allergic skin reaction.

H335 May cause respiratory irritation.

H411 Toxic to aquatic life with long lasting effects.

· **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.

P405 Store locked up.

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: 590-86-3 3-Methylbutyraldehyde

· **Identification number(s)**

· **EC number:** 209-691-5

· **Acute toxicity estimate (ATE) values** LD50 dermal: 2,534 mg/kg

**SECTION 4: First aid measures**

· **4.1 Description of first aid measures**

· **General information:** Immediately remove any clothing soiled by the product.

· **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:** If symptoms persist consult doctor.

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- **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.

**SECTION 5: Firefighting measures**

- **5.1 Extinguishing media**
- **Suitable extinguishing agents:**  
 CO<sub>2</sub>, 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 product to reach sewage system or any water course.  
 Inform respective authorities in case of seepage into water course or sewage system.  
 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**  
 Ensure good ventilation/exhaustion at the workplace.  
 Prevent formation of aerosols.
- **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:** Store in a cool location.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:**  
 Keep container tightly sealed.  
 Store in cool, dry conditions in well sealed receptacles.

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- **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.
- **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:**  
 In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.
- **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: 86.13 g/mol
- **Physical state** Fluid
- **Colour:** According to product specification
- **Odour:** According to product specification

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· <b>Odour threshold:</b>	Not determined.
· <b>Melting point/freezing point:</b>	-51 °C
· <b>Boiling point or initial boiling point and boiling range</b>	90 °C
· <b>Flammability</b>	Highly flammable.
· <b>Lower and upper explosion limit</b>	
· <b>Lower:</b>	1.7 Vol %
· <b>Upper:</b>	6.8 Vol %
· <b>Flash point:</b>	0.5 °C
· <b>Decomposition temperature:</b>	Not determined.
· <b>pH</b>	Not determined.
· <b>Viscosity:</b>	
· <b>Kinematic viscosity</b>	Not determined.
· <b>Dynamic:</b>	Not determined.
· <b>Solubility</b>	
· <b>water:</b>	Not miscible or difficult to mix.
· <b>Partition coefficient n-octanol/water (log value)</b>	Not determined.
· <b>Vapour pressure at 20 °C:</b>	61 hPa
· <b>Density and/or relative density</b>	
· <b>Density at 20 °C:</b>	0.803 g/cm <sup>3</sup>
· <b>Relative density</b>	Not determined.
· <b>Refractive Index</b>	
· <b>Vapour density</b>	Not determined.

· <b>9.2 Other information</b>	
· <b>Appearance:</b>	
· <b>Form:</b>	Liquid
· <b>Important information on protection of health and environment, and on safety.</b>	
· <b>Ignition temperature:</b>	Not determined.
· <b>Explosive properties:</b>	Product is not explosive. However, formation of explosive air/vapour mixtures are possible.
· <b>Solvent content:</b>	
· <b>VOC (EC)</b>	0.00 %
· <b>Change in condition</b>	
· <b>Evaporation rate</b>	Not determined.

· <b>Information with regard to physical hazard classes</b>	
· <b>Explosives</b>	Void
· <b>Flammable gases</b>	Void
· <b>Aerosols</b>	Void
· <b>Oxidising gases</b>	Void
· <b>Gases under pressure</b>	Void
· <b>Flammable liquids</b>	Highly flammable liquid and vapour.
· <b>Flammable solids</b>	Void
· <b>Self-reactive substances and mixtures</b>	Void
· <b>Pyrophoric liquids</b>	Void
· <b>Pyrophoric solids</b>	Void
· <b>Self-heating substances and mixtures</b>	Void

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- |   |      |
|---|------|
| · 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.
- **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** Based on available data, the classification criteria are not met.

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

CAS: 590-86-3 3-Methylbutyraldehyde

Oral	LD50	5,600 mg/kg (rat)
Dermal	LD50	2,534 mg/kg (ATE)
		3,180 mg/kg (rabbit)

- **Skin corrosion/irritation** Based on available data, the classification criteria are not met.
- **Serious eye damage/irritation** Causes serious eye irritation.
- **Respiratory or skin sensitisation** May cause an allergic skin reaction.
- **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** May cause respiratory irritation.
- **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.

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- **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.
- **12.7 Other adverse effects**
- **Remark:** Toxic for fish
- **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.  
Also poisonous for fish and plankton in water bodies.  
Toxic for aquatic organisms

### 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"> <li>· <b>14.1 UN number or ID number</b></li> <li>· <b>ADR, IMDG, IATA</b></li> </ul>                   | <p style="text-align: center;">UN2058</p>  |
| <ul style="list-style-type: none"> <li>· <b>14.2 UN proper shipping name</b></li> <li>· <b>ADR</b></li> <li>· <b>IMDG, IATA</b></li> </ul> | <p>2058 VALERALDEHYDE, ENVIRONMENTALLY HAZARDOUS<br/>VALERALDEHYDE</p>   |
| <ul style="list-style-type: none"> <li>· <b>14.3 Transport hazard class(es)</b></li> <li>· <b>ADR</b></li> </ul>                           | <div style="display: flex; align-items: center; gap: 10px;">   </div> <p style="margin-top: 10px;">· <b>Class</b> 3 (F1) Flammable liquids.<br/>· <b>Label</b> 3</p> |
| <ul style="list-style-type: none"> <li>· <b>IMDG, IATA</b></li> </ul>  | <div style="display: flex; align-items: center; gap: 10px;">  </div> <p style="margin-top: 10px;">· <b>Class</b> 3 Flammable liquids.</p>   |

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· Label	3
· 14.4 Packing group · ADR, IMDG, IATA	II
· 14.5 Environmental hazards: · Marine pollutant: · Special marking (ADR):	No Symbol (fish and tree)
· 14.6 Special precautions for user · Hazard identification number (Kemler code): · EMS Number: · Stowage Category	Warning: Flammable liquids. 33 F-E,S-D B
· 14.7 Maritime transport in bulk according to IMO instruments	Not applicable.
· Transport/Additional information:	
· ADR · Limited quantities (LQ) · Excepted quantities (EQ)	1L Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· Transport category · Tunnel restriction code	2 D/E
· IMDG · Limited quantities (LQ) · Excepted quantities (EQ)	1L Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· UN "Model Regulation":	UN 2058 VALERALDEHYDE, 3, II, ENVIRONMENTALLY HAZARDOUS

**SECTION 15: Regulatory information**

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

· Poisons Act

· Regulated explosives precursors

Substance is not listed.

· Regulated poisons

Substance is not listed.

· Reportable explosives precursors

Substance is not listed.

· Reportable poisons

Substance is not listed.

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

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

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· **Hazard pictograms**



GHS02 GHS07 GHS09

· **Signal word** Danger

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

3-Methylbutyraldehyde

· **Hazard statements**

H225 Highly flammable liquid and vapour.

H319 Causes serious eye irritation.

H317 May cause an allergic skin reaction.

H335 May cause respiratory irritation.

H411 Toxic to aquatic life with long lasting effects.

· **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.

P405 Store locked up.

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**

E2 Hazardous to the Aquatic Environment

P5c FLAMMABLE LIQUIDS

· **Qualifying quantity (tonnes) for the application of lower-tier requirements** 200 t

· **Qualifying quantity (tonnes) for the application of upper-tier requirements** 500 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.

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· **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

· **Date of previous version:** 29.09.2022

· **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. 2: Flammable liquids – Category 2

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

Skin Sens. 1B: Skin sensitisation – Category 1B

STOT SE 3: Specific target organ toxicity (single exposure) – Category 3

Aquatic Chronic 2: Hazardous to the aquatic environment - long-term aquatic hazard – Category 2

GB