

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision  
Supersedes Version

4 .00  
3 .00\*\*\*

Revision Date  
Issuing date

23-Jun-2017  
23-Jun-2017

## SECTION 1: Identification

### 1.1. Product identifier

Identification of the  
substance/preparation

**Isovaleraldehyde**

Chemical Name  
CAS-No

3-Methylbutanal\*\*\*  
590-86-3

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

Use of the Substance /  
Preparation

Intermediate

Uses advised against

None

### 1.3. Details of the supplier of the safety data sheet

Supplier

**OXEA Corporation**  
1505 West LBJ Freeway, Suite 400  
Dallas, TX 75234  
USA  
Phone: +1 972 481 2700

Product Information

Product Stewardship  
FAX: +49 (0)208 693 2053  
email: psq@oxea-chemicals.com

### 1.4. Emergency telephone number

Emergency telephone number

in USA, call 800 424 9300  
outside USA, call 703 527 3887, collect calls accepted  
available 24/7

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

This substance is classified in accordance with paragraph (d) of §1910.1200 (GHS-US classification).

Serious eye damage/eye irritation Category 2A, H319  
Skin sensitization Category 1, H317  
Target Organ Systemic Toxicant - Single exposure Category 3, H335  
Flammable liquid Category 2, H225  
Environmental hazard Aquatic Chronic 2; H411; Aquatic Acute 2; H401

OSHA Specified Hazards

Not applicable.

Emergency telephone number  
1 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

## 2.2. Label elements

Labeling according to §1910.1200 (GHS-US labeling).

### Hazard symbol(s)



### Signal word

**Danger**

### Hazard statements

H225: Highly flammable liquid and vapor.  
H319: Causes serious eye irritation.  
H317: May cause an allergic skin reaction.  
H335: May cause respiratory irritation.  
H401: Toxic to aquatic life  
H411: Toxic to aquatic life with long lasting effects.

### Precautionary statements

#### Prevention

P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P233: Keep container tightly closed.  
P240: Ground and bond container and receiving equipment.  
P241: Use explosion-proof electrical/ ventilating/ lighting equipment.  
P242: Use non-sparking tools.  
P243: Take action to prevent static discharges.  
P280: Wear protective gloves/eye protection/face protection.  
P264: Wash hands thoroughly after handling.  
P261: Avoid breathing gas/mist/vapours.  
P271: Use only outdoors or in a well ventilated area.  
P272: Contaminated work clothing must not be allowed out of the workplace.  
P273: Avoid release to the environment.

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

<b>Response</b>	P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower. P333 + P313: If skin irritation or rash occurs: Get medical advice/attention. P302 + P352: IF ON SKIN: Wash with plenty of soap and water. P363: Wash contaminated clothing before reuse. P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337 + P313: If eye irritation persists: Get medical advice/ attention. P304 + P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P312: Call a POISON CENTRE/doctor if you feel unwell. P391: Collect spillage.
<b>Storage</b>	P403 + P235: Store in a well ventilated place. Keep cool. P405: Store locked up.
<b>Disposal</b>	P501: Dispose of contents/container in accordance with local regulation.

## 2.3. Other hazards

Vapours may form explosive mixture with air  
Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback  
Components of the product may be absorbed into the body by inhalation, ingestion and through the skin

## SECTION 3: Composition / information on ingredients

### 3.1. Substances

Component	CAS-No	Concentration (%)
Isovaleraldehyde	590-86-3	> 99,0

#### Remarks

3-Methylbutanal.

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

#### Inhalation

Keep at rest. Aerate with fresh air. When symptoms persist or in all cases of doubt seek medical advice.

#### Skin

Wash off immediately with soap and plenty of water. When symptoms persist or in all cases of doubt seek medical advice.

#### Eyes

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses. Obtain medical attention.

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

## Ingestion

Do not induce vomiting without medical advice. Call a physician immediately.

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

### Main symptoms

shortness of breath, vomiting, headache, nausea.

### Special hazard

Lung oedema, Lung irritation.

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

### General advice

Remove contaminated, soaked clothing immediately and dispose of safely. First aider needs to protect himself.

Treat symptomatically. In case of lung irritation, first treatment with cortisone spray.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

alcohol-resistant foam, dry chemical, carbon dioxide (CO<sub>2</sub>), water spray

#### Unsuitable Extinguishing Media

Do not use a solid water stream as it may scatter and spread fire.

### 5.2. Special hazards arising from the substance or mixture

Under conditions giving incomplete combustion, hazardous gases produced may consist of:

carbon monoxide (CO)

carbon dioxide (CO<sub>2</sub>)

Combustion gases of organic materials must in principle be graded as inhalation poisons

Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback

Vapours may form explosive mixture with air

### 5.3. Advice for firefighters

#### Special protective equipment for firefighters

Fire fighter protection should include a self-contained breathing apparatus (NIOSH-approved or EN 133) and full fire-fighting turn out gear.

#### Precautions for firefighting

Keep people away from and upwind of fire. Cool containers / tanks with water spray. Dike and collect water used to fight fire. Water run-off can cause environmental damage.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

Emergency telephone number  
4 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

For non-emergency personnel: For personal protective equipment see section 8. Avoid contact with skin and eyes. Avoid breathing vapors or mists. Keep people away from and upwind of spill/leak. Ensure adequate ventilation, especially in confined areas. Keep away from heat and sources of ignition.  
For emergency responders: Personal protection see section 8.\*\*\*

## 6.2. Environmental precautions

Prevent further leakage or spillage. Do not discharge product into the aquatic environment without pretreatment (biological treatment plant). Water runoff can cause environmental damage.

## 6.3. Methods and material for containment and cleaning up

### Methods for containment

Stop the flow of material, if possible without risk. Dike spilled material, where this is possible.

### Methods for cleaning up

Soak up with inert absorbent material. DO NOT use combustible materials such as sawdust. Keep in suitable, closed containers for disposal. If liquid has been spilt in large quantities clean up promptly by scoop or vacuum. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours).

## 6.4. Reference to other sections

For personal protective equipment see section 8.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Advice on safe handling

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. Provide sufficient air exchange and/or exhaust in work rooms. Refill and handle product only in closed system. Do not use compressed air for filling, discharging or handling.

#### Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

#### Advice on the protection of the environment

See Section 8: Environmental exposure controls.

#### Incompatible products

acids and bases  
amines  
oxidizing agents

### 7.2. Conditions for safe storage, including any incompatibilities

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

## Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge (which might cause ignition of organic vapours). In case of fire, emergency cooling with water spray should be available. Ground and bond containers when transferring material. Vapour is heavier than air and can travel considerable distance to a source of ignition and flashback. Vapours may form explosive mixture with air.

## Technical measures/Storage conditions

Keep containers tightly closed in a cool, well-ventilated place. Handle and open container with care. Handle under nitrogen, protect from moisture. Store at temperatures not exceeding 38 °C/ 100 °F.

## Suitable material

stainless steel

## Unsuitable material

mild steel

## SECTION 8: Exposure controls / personal protection

### 8.1. Control parameters

#### Exposure limits United States of America

No exposure limits established regarding ACGIH, OSHA Z-1 and OSHA Z-2.

### 8.2. Exposure controls

#### Appropriate Engineering controls

General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

#### Individual protection measures, such as personal protective equipment

##### General industrial hygiene practice

Avoid contact with skin, eyes and clothing. Do not breathe vapours or spray mist. Ensure that eyewash stations and safety showers are close to the workstation location.

##### Hygiene measures

When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

##### Eye protection

Tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face.

##### Hand protection

Wear protective gloves. Recommendations are listed below. Other protective material may be used, depending on the situation, if adequate degradation and permeation data is available. If other chemicals are used in conjunction with this chemical, material selection should be based on protection for all chemicals present.

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

**Suitable material** butyl-rubber  
**Evaluation** according to EN 374: level 3  
**Glove thickness** approx 0.3 mm  
**Break through time** approx 60 min

**Suitable material** polyvinylchloride  
**Evaluation** Information derived from practical experience  
**Glove thickness** approx 0.8 mm

## Skin and body protection

Impervious clothing. Wear face-shield and protective suit for abnormal processing problems.

## Respiratory protection

Respirator with filter for organic vapour. Use the indicated respiratory protection if the occupational exposure limit is exceeded and/or in case of product release (dust). Equipment should conform to NIOSH.

## Environmental exposure controls

If possible use in closed systems. If leakage can not be prevented, the substance needs to be suck off at the emersion point, if possible without danger. If recycling is not practicable, dispose of in compliance with local regulations. Inform the responsible authorities in case of leakage into the atmosphere, or of entry into waterways, soil or drains.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

**Appearance** liquid  
**Colour** colourless  
**Odour** strong  
**Odour threshold** 0,1 - 2 ppb  
**pH** 3,1 (15 g/l in water @ 20 °C (68 °F))  
**Melting point/range** < -130 °F (< -90 °C) (Pour point)  
**Boiling point/range** 198 °F (92 °C) @ 1 atm (101,3 kPa)  
**Flash point** 33 °F (0,5 °C)  
**Method** EU A.9  
**Evaporation rate** No data available  
**Flammability (solid, gas)** Does not apply, the substance is a liquid  
**Lower explosion limit** No data available  
**Upper explosion limit** No data available

#### Vapour pressure

Values [hPa]	Values [kPa]	Values [atm]	@ °C	@ °F	Method
75	7,5	0,074	20	68	
255	25,5	0,252	50	122	

**Vapour density** 2,96 (Air = 1) @ 20 °C (68 °F)

#### Relative density

Values	@ °C	@ °F	Method
0,797	20	68	DIN 51757

**Solubility** 15 g/l @ 20 °C (68 °F), in water, OECD 105\*\*\*

Emergency telephone number  
7 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

log Pow	1,5 (measured) OECD 117
Autoignition temperature	410 °F (210 °C)
Method	DIN 51794
Decomposition temperature	No data available
Viscosity	0,69 mm <sup>2</sup> /s @ 68 °F (20 °C)***
Method	OECD 114, kinematic***

## 9.2. Other information

Molecular weight	86,13
Molecular formula	C5 H10 O
Oxidizing properties	Does not apply, substance is not oxidising. There are no chemical groups associated with oxidizing properties
Refractive Index	1,387 @ 68 °F (20 °C)
Explosive properties	Does not apply, substance is not explosive. There are no chemical groups associated with explosive properties
Surface tension	46,1 mN/m (1 g/l @ 20°C (68°F)), OECD 115***

## SECTION 10: Stability and Reactivity

### 10.1. Reactivity

The reactivity of the product corresponds to the typical reactivity shown by the substance group as described in any text book on organic chemistry.

### 10.2. Chemical stability

Stable under recommended storage conditions.

### 10.3. Possibility of hazardous reactions

Hazardous polymerisation may occur. Polymerization is a highly exothermic reaction and may generate sufficient heat to cause thermal decomposition and/or rupture containers. May form explosive peroxides. When finely distributed, self-ignition is possible. Vapours may form explosive mixture with air.

### 10.4. Conditions to avoid

Avoid contact with heat, sparks, open flame and static discharge. Avoid any source of ignition.

### 10.5. Incompatible materials

bases, amines, acids, oxidizing agents.

### 10.6. Hazardous decomposition products

No decomposition if stored and applied as directed.\*\*\*

## SECTION 11: Toxicological information



# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

## 11.1. Information on toxicological effects

Likely routes of exposure Inhalation, Eye contact, Skin contact, Ingestion

### Isovaleraldehyde, CAS: 590-86-3

#### Main symptoms

shortness of breath, vomiting, nausea, headache.

#### Target Organ Systemic Toxicant - Single exposure

The available data lead to the classification given in section 2

#### Target Organ Systemic Toxicant - Repeated exposure

Based on available data, the classification criteria are not met for:

STOT RE

Acute toxicity				
Isovaleraldehyde (590-86-3)				
Routes of Exposure	Endpoint	Values	Species	Method
Oral	LD50	~ 5740 mg/kg	rat, male/female	OECD 401
Dermal	LD50	2534 mg/kg	rabbit	OECD 402
Inhalative	LC50	42,7 mg/l (4h)	rat	OECD 403

### Isovaleraldehyde, CAS: 590-86-3

#### Assessment

Based on available data, the classification criteria are not met for:

Acute oral toxicity

Acute dermal toxicity

Acute inhalation toxicity

Irritation and corrosion				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Result	Method	
Skin	rabbit	Mild skin irritation	OECD 404	4h
Eyes	rabbit	irritating		
Respiratory tract***	mouse***	RD50: 757-1000 ppm***		

### Isovaleraldehyde, CAS: 590-86-3

#### Assessment

The available data lead to the classification given in section 2\*\*\*

Sensitization				
Isovaleraldehyde (590-86-3)				
Target Organ Effects	Species	Evaluation	Method	
Skin	mouse guinea pig***	sensitizing***		read across

### Isovaleraldehyde, CAS: 590-86-3

#### Assessment

The available data lead to a classification as skin sensitizer (see section 2)

For respiratory sensitization, no data are available

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

Subacute, subchronic and prolonged toxicity				
Isovaleraldehyde (590-86-3)				
Type	Dose	Species	Method	
no data available***				

Carcinogenicity, Mutagenicity, Reproductive toxicity					
Isovaleraldehyde (590-86-3)					
Type	Dose	Species	Evaluation	Method	
Mutagenicity		human lymphocytes	positive (without metabolic activation)	Similar to: OECD 479 (SCE)***	In vitro study
Mutagenicity		Salmonella typhimurium	negative	OECD 471 (Ames)	read across
Mutagenicity		mouse	negative	OECD 474 Chromosomal Aberration***	
Carcinogenicity	LOAEC: 500 ppm	rat, male/female	negative***	OECD 451, Inhalative	read across
Carcinogenicity	LOAEC: 500 ppm	mouse male/female***	negative***	OECD 451, Inhalative	read across
Reproductive toxicity***	No data available***				

## Isovaleraldehyde, CAS: 590-86-3

### CMR Classification

The available data on CMR properties are summarized in the table above. They do not indicate a classification into categories 1A or 1B

### Evaluation

Did not show carcinogenic or mutagenic effects in animal experiments\*\*\*

## Isovaleraldehyde, CAS: 590-86-3

### Aspiration toxicity

According to experience not expected

### Other adverse effects

Components of the product may be absorbed into the body by inhalation, ingestion and through the skin.

### Note

Handle in accordance with good industrial hygiene and safety practice. Further details on substance data can be found in the registration dossier under the following link:

<http://echa.europa.eu/information-on-chemicals/registered-substances>.

## SECTION 12: Ecological information

### 12.1. Toxicity

Acute aquatic toxicity			
Isovaleraldehyde (590-86-3)			
Species	Exposure time	Dose	Method
Daphnia magna (Water flea)	48h	EC50: 177 mg/l	84/449/EEC C.2

Emergency telephone number  
10 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

Pimephales promelas (fathead minnow)	96h	LC50: 3,25 mg/l	OECD 203
Desmodesmus subspicatus	72h	EC50: 80 mg/l (Biomass)	DIN 38412, part 9
Desmodesmus subspicatus	72h	EC50: 112,78 mg/l (Growth rate)	DIN 38412, part 9

## Long term toxicity

### Isovaleraldehyde (590-86-3)

Type	Species	Dose	Method	
Aquatic toxicity***	Desmodesmus subspicatus***	EC10: 32.62 mg/l (72 h) Biomass***	DIN 38412 / part 9***	
Aquatic toxicity***	Desmodesmus subspicatus***	EC10: 71,89 mg/l (72 h) Growth inhibition***	DIN 38412 / part 9***	

## 12.2. Persistence and degradability

### Isovaleraldehyde, CAS: 590-86-3

#### Biodegradation

50 % (28 d), Sewage, aerobic, OECD 301 D.

#### Abiotic Degradation

### Isovaleraldehyde (590-86-3)

Type	Result	Method
Hydrolysis***	No data available***	
Photolysis***	No data available***	

## 12.3. Bioaccumulative potential

### Isovaleraldehyde (590-86-3)

Type	Result	Method
log Pow***	1,5***	OECD 117***
BCF***	No data available***	

## 12.4. Mobility in soil

No data available

### Isovaleraldehyde (590-86-3)

Type	Result	Method
Surface tension***	46,1 mN/m (1 g/l @ 20°C (68°F))***	
Adsorption/Desorption***	no data available***	
Distribution to environmental compartments***	no data available***	

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

## 12.5. Results of PBT and vPvB assessment

Isovaleraldehyde, CAS: 590-86-3  
PBT and vPvB assessment  
Not required\*\*\*

## 12.6. Other adverse effects

Isovaleraldehyde, CAS: 590-86-3  
No data available

### Note

Avoid release to the environment.

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Product Information

Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.

#### Uncleaned empty packaging

Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

## SECTION 14: Transport information

### D.O.T. (49CFR)

14.1. UN number	UN 2058
14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II
14.5. Environmental hazards	no
14.6. Special precautions for user	
Emergency Response Guide	129

### ICAO-TI / IATA-DGR

14.1. UN number	UN 2058
14.2. UN proper shipping name	Valeraldehyde
14.3. Transport hazard class(es)	3
14.4. Packing group	II

Emergency telephone number  
12 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

14.5. Environmental hazards no  
14.6. Special precautions for user no data available

## IMDG

14.1. UN number UN 2058  
14.2. UN proper shipping name Valeraldehyde  
14.3. Transport hazard class(es) 3  
14.4. Packing group II  
14.5. Environmental hazards no  
14.6. Special precautions for user  
EmS F-E, S-D

## 14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Product name Valeraldehyde  
Ship type 3  
Pollution category Y

## **SECTION 15: Regulatory information**

### **Federal and State Regulations**

Components of the product are listed in the quoted regulations. For details please refer to the regulations directly. This list is not exhaustive, please check for other applicable regulations.

#### **Federal Regulations**

This product is listed on the TSCA inventory

#### **Isovaleraldehyde, CAS: 590-86-3**

CERCLA Hazardous Substance  
CERCLA RQ 100 LBS

#### **State Regulations**

#### **Isovaleraldehyde, CAS: 590-86-3**

IL Chemical Safety Act  
MA RTK List  
NY RTK List  
PA RTK List

#### **International Inventories**

#### **Isovaleraldehyde, CAS: 590-86-3**

AICS (AU)  
DSL (CA)  
IECSC (CN)  
EC-No. 2096915 (EU)

Emergency telephone number  
13 / 14

in USA, call 800 424 9300; outside USA, call USA 703 527 3887, collect calls accepted  
USA (A-US)

# SAFETY DATA SHEET



Isovaleraldehyde  
10150

Version / Revision 4 .00

ENCS (2)-494 (JP)  
ISHL (2)-494 (JP)  
KECI KE-23536 (KR)  
INSQ (MX)  
PICCS (PH)  
TSCA (US)  
NZIoC (NZ)  
TCSI (TW)

## SECTION 16: Other information

Revision Date 23-Jun-2017  
Issuing date 23-Jun-2017

### Hazard Rating Systems

#### **NFPA (National Fire Protection Association)**

Health Hazard	1
Fire Hazard	3
Reactivity	0

#### **HMIS (Hazardous Material Information System)**

Health Hazard	1
Flammability	3
Physical Hazard	0

### **Training advice**

For effective first-aid, special training / education is needed.

### **Sources of key data used to compile the datasheet**

Information contained in this safety data sheet is based on Oxea owned data and public sources deemed valid or acceptable. The absence of data elements required by OSHA, ANSI or Annex II, Regulation 1907/2006/EC indicates, that no data meeting these requirements is available.

### **Further information for the safety data sheet**

Changes against the previous version are marked by \*\*\*. Observe national and local legal requirements. For more information, other material safety data sheets or technical data sheets please consult the Oxea homepage ([www.oxea-chemicals.com](http://www.oxea-chemicals.com)).

### **Disclaimer**

**For industrial use only.** The information contained herein is accurate to the best of our knowledge. We do not suggest or guarantee that any hazards listed herein are the only ones which exist. Oxea makes no warranty of any kind, express or implied, concerning the safe use of this material in your process or in combination with other substances. User has the sole responsibility to determine the suitability of the materials for any use and the manner of use contemplated. User must meet all applicable safety and health standards.

**End of Safety Data Sheet**