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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Isovaleraldehyde

Product Number : 146455

Brand : Aldrich

CAS-No. : 590-86-3

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225

Eye irritation (Category 2A), H319

Skin sensitisation (Category 1), H317

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Danger

Hazard statement(s)

H225

Highly flammable liquid and vapour.

H317

May cause an allergic skin reaction.

H319

Causes serious eye irritation.

H335

May cause respiratory irritation.

H411

Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

|                    |  |
|--------------------|--|
| P241               | Use explosion-proof electrical/ ventilating/ lighting/ equipment.  |
| P242               | Use only non-sparking tools.   |
| P243               | Take precautionary measures against static discharge.  |
| P261               | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.   |
| P264               | Wash skin thoroughly after handling.   |
| P271               | Use only outdoors or in a well-ventilated area.  |
| P272               | Contaminated work clothing should not be allowed out of the workplace.   |
| P273               | Avoid release to the environment.  |
| P280               | Wear protective gloves/ eye protection/ face protection.   |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.                              |
| P304 + P340 + P312 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell.       |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P333 + P313        | If skin irritation or rash occurs: Get medical advice/ attention.  |
| P337 + P313        | If eye irritation persists: Get medical advice/ attention.   |
| P363               | Wash contaminated clothing before reuse.   |
| P370 + P378        | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.   |
| P391               | Collect spillage.  |
| P403 + P233        | Store in a well-ventilated place. Keep container tightly closed.   |
| P403 + P235        | Store in a well-ventilated place. Keep cool.   |
| P405               | Store locked up.   |
| P501               | Dispose of contents/ container to an approved waste disposal plant.  |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Stench.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |                                    |
|------------------|------------------------------------|
| Synonyms         | : 3-Methylbutyraldehyde            |
| Formula          | : C <sub>5</sub> H <sub>10</sub> O |
| Molecular weight | : 86.13 g/mol                      |
| CAS-No.          | : 590-86-3                         |
| EC-No.           | : 209-691-5                        |

#### Hazardous components

| Component        | Classification   | Concentration |
|------------------|--|---------------|
| Isovaleraldehyde | Flam. Liq. 2; Eye Irrit. 2A; Skin Sens. 1; STOT SE 3; Aquatic Acute 2; Aquatic Chronic 2; H225, H317, H319, H335, H411 | 90 - 100 %    |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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**5. FIREFIGHTING MEASURES****5.1 Extinguishing media****Suitable extinguishing media**

Dry powder Dry sand

**Unsuitable extinguishing media**

Do NOT use water jet.

**5.2 Special hazards arising from the substance or mixture**

No data available

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

**6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

**6.4 Reference to other sections**

For disposal see section 13.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities**

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature 2 - 8 °C

Handle and store under inert gas. Air and light sensitive. Stench.

Storage class (TRGS 510): 3: Flammable liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

Hazardous components without workplace control parameters

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 30 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

##### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                    |   |
|--------------------|---|
| a) Appearance      | Form: clear, liquid<br>Colour: colourless |
| b) Odour           | unpleasant                                |
| c) Odour Threshold | No data available                         |
| d) pH              | No data available                         |

|   |   |
|---|---|
| e) Melting point/freezing point                 | Freezing point: < -90 °C (< -130 °F)                        |
| f) Initial boiling point and boiling range      | 90 °C (194 °F) - lit.                                       |
| g) Flash point                                  | -5 °C (23 °F) - closed cup                                  |
| h) Evaporation rate                             | No data available   |
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | No data available   |
| k) Vapour pressure                              | 40 hPa (30 mmHg) at 20 °C (68 °F)                           |
| l) Vapour density                               | 2.97 - (Air = 1.0)  |
| m) Relative density                             | 0.803 g/cm <sup>3</sup> at 25 °C (77 °F)                    |
| n) Water solubility                             | 15 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - soluble |
| o) Partition coefficient: n-octanol/water       | log Pow: 1.5 at 25 °C (77 °F)                               |
| p) Auto-ignition temperature                    | 210 °C (410 °F) at 1,020 hPa (765 mmHg)                     |
| q) Decomposition temperature                    | No data available   |
| r) Viscosity                                    | 0.69 mm <sup>2</sup> /s at 20 °C (68 °F) -                  |
| s) Explosive properties                         | No data available   |
| t) Oxidizing properties                         | No data available   |

## 9.2 Other safety information

Relative vapour density 2.97 - (Air = 1.0)

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Oxidizing agents, Strong bases, Strong reducing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 5,600 mg/kg

Remarks: Behavioral: Somnolence (general depressed activity).

LD50 Oral - Rat - 5,740 mg/kg  
(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - 42,700 mg/m<sup>3</sup>

Remarks: Behavioral: Altered sleep time (including change in righting reflex). Gastrointestinal: Changes in structure or function of salivary glands.

LD50 Dermal - Rabbit - 2,534 mg/kg

Remarks: Liver: Other changes. Prolonged skin contact may cause skin irritation and/or dermatitis.

No data available

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: Mild skin irritation - 24 h

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Irritating to eyes. - 8 d

#### **Respiratory or skin sensitisation**

The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### **Reproductive toxicity**

No data available

No data available

#### **Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation. - Respiratory system

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

#### **Additional Information**

RTECS: ES3450000

Nausea, Headache, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **12. ECOLOGICAL INFORMATION**

### **12.1 Toxicity**

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 3.25 mg/l - 96 h

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 177 mg/l - 48 h

Toxicity to algae ErC50 - Desmodesmus subspicatus (green algae) - 113 mg/l - 72 h

### **12.2 Persistence and degradability**

Biodegradability Result: 50 % - Not readily biodegradable.

(OECD Test Guideline 301D)

**12.3 Bioaccumulative potential**

Does not bioaccumulate.

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life with long lasting effects.

No data available

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**13. DISPOSAL CONSIDERATIONS**

**13.1 Waste treatment methods**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION**

**DOT (US)**

UN number: 1989      Class: 3      Packing group: II  
Proper shipping name: Aldehydes, n.o.s.  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1989      Class: 3      Packing group: II      EMS-No: F-E, S-D  
Proper shipping name: ALDEHYDES, N.O.S. (Isovaleraldehyde)

**IATA**

UN number: 1989      Class: 3      Packing group: II  
Proper shipping name: Aldehydes, n.o.s. (Isovaleraldehyde)

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**15. REGULATORY INFORMATION**

**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard

**Massachusetts Right To Know Components**

|                  |                     |                             |
|------------------|---------------------|-----------------------------|
| Isovaleraldehyde | CAS-No.<br>590-86-3 | Revision Date<br>1993-04-24 |
|------------------|---------------------|-----------------------------|

**Pennsylvania Right To Know Components**

|                  |                     |                             |
|------------------|---------------------|-----------------------------|
| Isovaleraldehyde | CAS-No.<br>590-86-3 | Revision Date<br>1993-04-24 |
|------------------|---------------------|-----------------------------|

|                  |                     |                             |
|------------------|---------------------|-----------------------------|
| Isovaleraldehyde | CAS-No.<br>590-86-3 | Revision Date<br>1993-04-24 |
|------------------|---------------------|-----------------------------|

## New Jersey Right To Know Components

Isovaleraldehyde

CAS-No.  
590-86-3

Revision Date  
1993-04-24

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

|                 |  |
|-----------------|--|
| Aquatic Acute   | Acute aquatic toxicity                           |
| Aquatic Chronic | Chronic aquatic toxicity                         |
| Eye Irrit.      | Eye irritation                                   |
| Flam. Liq.      | Flammable liquids                                |
| H225            | Highly flammable liquid and vapour.              |
| H317            | May cause an allergic skin reaction.             |
| H319            | Causes serious eye irritation.                   |
| H335            | May cause respiratory irritation.                |
| H401            | Toxic to aquatic life.                           |
| H411            | Toxic to aquatic life with long lasting effects. |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         |   |
| Chronic Health Hazard: | * |
| Flammability:          | 3 |
| Physical Hazard        |   |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     |   |
| Fire Hazard:       | 3 |
| Reactivity Hazard: |   |

### Further information

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### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 4.9

Revision Date: 03/23/2018

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