

# SAFETY DATA SHEET

Version 6.7  
Revision Date 08/05/2024  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 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 sensitization (Category 1), H317  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (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 Statements

H225 Highly flammable liquid and vapor.  
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 Statements

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 mist or vapors.  
P264 Wash skin thoroughly after handling.  
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.  
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.

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## SECTION 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

Component	Classification	Concentration
<b>Isovaleric aldehyde</b>		
	Flam. Liq. 2; Eye Irrit. 2A; Skin Sens. 1; STOT SE 3; Aquatic Acute 2; Aquatic Chronic 2; H225, H319, H317, H335, H401, H411	<= 100 %

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

No data available

### 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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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Foam Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides  
Combustible.

### 5.3 Advice for firefighters

No data available

## 5.4 Further information

No data available

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## SECTION 6: Accidental release measures

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

For personal protection see section 8.

### 6.2 Environmental precautions

No data available

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

No data available

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

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

**Storage stability** Recommended storage temperature

2 - 8 °C

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

#### **Storage class**

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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### **Personal protective equipment**

##### **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 EC 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.

### **Control of environmental exposure**

Prevent product from entering drains.

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## **SECTION 9: Physical and chemical properties**

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

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	unpleasant
c) Odor 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	0.5 °C (32.9 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 6.8 %(V) Lower explosion limit: 1.7 %(V)
k) Vapor pressure	40 hPa at 20 °C (68 °F)
l) Vapor density	2.97 - (Air = 1.0)
m) Density	0.803 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
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) - Bioaccumulation is not expected.
p) Autoignition	210 °C (410 °F) at 1,020 hPa

- temperature
- q) Decomposition temperature No data available
- r) Viscosity 0.69 mm<sup>2</sup>/s at 20 °C (68 °F) - OECD Test Guideline 114 -
- s) Explosive properties No data available
- t) Oxidizing properties none

## 9.2 Other safety information

Relative vapor density 2.97 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
alkalines  
Oxidizing agents  
strong reducing agents

### 10.4 Conditions to avoid

Air

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

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

LC50 Inhalation - Rat - 4 h - 42.7 mg/l - vapor

(OECD Test Guideline 403)

Inhalation: Irritating to respiratory system.

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

LD50 Dermal - Rabbit - 2,534 mg/kg  
(OECD Test Guideline 402)

Remarks: Liver:Other changes.

Prolonged skin contact may cause skin irritation and/or dermatitis.  
(RTECS)

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

Skin - Rabbit

Result: Mild skin irritation - 4 h  
(OECD Test Guideline 404)

Remarks: Irritations  
Dermatitis

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

Eyes - Rabbit

Result: Irritating to eyes. - 8 d

#### **Respiratory or skin sensitization**

May cause allergic skin reaction. (ECHA)

#### **Germ cell mutagenicity**

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

#### **Carcinogenicity**

IARC: No ingredient 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 ingredient 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

#### **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

### **11.2 Additional Information**

RTECS: ES3450000

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

After absorption of toxic quantities:

Headache  
Nausea  
Vomiting

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 3.25 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 177 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 112.78 mg/l - 72 h (DIN 38412)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 49.5 % - Not readily biodegradable. (OECD Test Guideline 301D)
Biochemical Oxygen Demand (BOD)	1,423 mg/g Remarks: (External MSDS)
Chemical Oxygen Demand (COD)	1,908 mg/g Remarks: (External MSDS)

### 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 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

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**SECTION 13: Disposal considerations****13.1 Waste treatment methods**

No data available

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**SECTION 14: Transport information****DOT (US)**

UN number: 2058 Class: 3 Packing group: II  
Proper shipping name: Valeraldehyde  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 2058 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: VALERALDEHYDE

**IATA**

UN number: 2058 Class: 3 Packing group: II  
Proper shipping name: Valeraldehyde

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : 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.

**US State Regulations****Massachusetts Right To Know**

Isovaleric aldehyde 590-86-3

**Pennsylvania Right To Know**

Isovaleric aldehyde 590-86-3

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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