

## 3-Methylbutyraldehyde-2,2-d<sub>2</sub>

### Section 1. Chemical product and company identifications

**Product code:** D-5269

**Chemical formula:** C<sub>5</sub>H<sub>8</sub>D<sub>2</sub>O

**CAS:** 352431-47-1

**CAS (unlabelled):** 590-86-3

**Synonyms:** Isovaleraldehyde, 3-Methylbutanal

**Supplier / Manufacturer:**

**C/D/N Isotopes Inc.**

88 Leacock Street

Pointe-Claire (Québec) H9R 1H1

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**In case of emergency:**

**TOXYSKAN HOTLINE: 1-855-780-0599**



### Section 2. Hazards identifications

**GHS (Globally Harmonized System of Classification and Labelling of Chemicals):**

**GHS Classification:**

- Flammable liquids (Category 2)
- Eye irritation (Category 2A)
- Skin sensitisation (Category 1)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system

**GHS Label elements:**

- Pictograms:  
- Signal word: Danger

**Hazards statement:**

- H225 Highly flammable liquid and vapour.
- H317 May cause an allergic skin reaction.
- H319 Causes serious eye irritation.
- H335 May cause respiratory irritation.

**Precautionary statement:**

- P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ 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.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P264 + P265 Wash your hands thoroughly after handling. Do not touch eyes.
- P271 Use only outdoors or in a well-ventilated area.
- P272 Contaminated work clothing should not be allowed out of the workplace
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- 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.
- P362 + P364 Take off contaminated clothing and wash it before reuse.
- P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- 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.

### **Section 3. Composition and information on ingredients**

<b><u>Name</u></b>	<b><u>CAS</u></b>	<b><u>Concentration %</u></b>
3-Methylbutyraldehyde-2,2-d <sub>2</sub>	352431-47-1	> 96

### **Section 4. First aid measures**

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

**Skin contact:** Wash off with soap and plenty of water. Consult a physician.

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

**Ingestion:** Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

**Indication of immediate medical attention and special treatment needed, if necessary:** No data available

**Most important symptoms and effects, both acute and delayed:** Redness, Sore throat, Cough.

### **Section 5. Firefighting measures**

**Flammability of the product:** Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides.

**Firefighting media and instructions:** Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Special protective equipment for firefighters:** Wear self-contained breathing apparatus for firefighting if necessary.

### **Section 6. Accidental release measures**

**Personal precautions:** Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition.

**Environmental precautions:** Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up:** Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

### **Section 7. Handling and storage**

**Handling:** Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking.

**Storage:** STORE REFRIGERATED. Adequate ventilation. Protect from heat and ignition sources. Protect from light. Protect from moisture.

### **Section 8. Exposure Controls, Personal Protections**

**Engineering controls:** Use mechanical exhaust or laboratory fumehood to avoid exposure.

**Eyes:** Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).

**Respiratory:** 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).

**Hands:** Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Skin/body:** Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

## **Section 9. Physical and chemical properties (unlabelled)**

**Molecular weight:** 86.13 g/mol  
**Physical status:** Liquid  
**Color:** Colorless  
**Odour:** Unpleasant  
**Density:** 0.803 g/cm<sup>3</sup>  
**Melting point:** -51 °C (-60 °F)  
**Boiling point:** 90 °C (194 °F)  
**Vapour pressure:** 40 hPa (30 mmHg) at 20 °C (68 °F)  
**Vapour density:** 2.97 (Air = 1)  
**Partition coefficient (octanol/water):** No data available  
**Water solubility:** 14 g/L  
**Lower explosion limit:** 1.4 Vol%  
**Upper explosion limit:** 5.6 Vol%  
**Auto-ignition temperature:** 210 °C (410 °F)  
**Flash point:** -5 °C (23 °F)

## **Section 10. Stability and reactivity**

**Stability and reactivity:** Stable under recommended storage conditions.  
**Incompatibility:** Oxidizing agents, strong bases, strong reducing agents.  
**Products of combustion:** Hazardous decomposition products formed under fire conditions: Carbon oxides.  
**Reactivity conditions:** Heat, flames and sparks.

## **Section 11. Toxicological information (unlabelled)**

**Toxicological data:** Isovaleraldehyde

### **Information on ingredients:**

<b>Name</b>	<b>CAS</b>	<b>LD<sub>50</sub></b>	<b>LC<sub>50</sub></b>
Isovaleraldehyde	590-86-3	Oral - Rat - 5,600 mg/kg Dermal - Rabbit - 2,560 mg/kg Oral - Mouse - 4,750 mg/kg	Inhalation - Rat - 4 h - 42,700 mg/m <sup>3</sup>

### **Potential acute effects**

- **Eyes:** Causes serious eye irritation.
- **Skin:** May cause skin irritation.
- **Inhalation:** May cause respiratory tract irritation.
- **Ingestion:** No data available.

### **Potential chronic effects**

- **Carcinogenic effects:** 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. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

## **Section 12. Ecological information**

### **Ecological data:**

<b>Name</b>	<b>Results</b>	<b>Species</b>	<b>Period</b>
Isovaleraldehyde	3.25 mg/l LC50 177 mg/l EC50	Pimephales promelas Daphnia magna	96 h 48 h

**Effects on environment:** An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
**Mobility:** No data available.  
**Environmental precautions:** No data available.  
**Persistence and degradability:** Result: 50 % - Not readily biodegradable. Method: OECD Test Guideline 301D.  
**Bioaccumulative potential:** Does not bioaccumulate.

## **Section 13. Disposal considerations**

**Waste disposal:** Contact a licensed professional waste disposal service to dispose of this material.

## **Section 14. Transportation information**

### **Classification DOT/IMDG/IATA label:**

**Shipping name:** Valeralehyde

**UN number:** UN2058

**Class:** 3

**Packaging group:** II

**Additional information:** None

## **Section 15. Regulatory information**

### **UNITED STATES: NFPA classification**



Health: 2  
Flammable: 3  
Reactivity: 0  
Special conditions: None

**Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous**

### **U.S. Federal regulations:**

**California proposition 65 requirements :** Not Listed

**SARA section 313 (specific toxic chemical listings) :** Not listed

**CERCLA reportable quantity :** Not listed

**Sections 302-304 reportable quantity :** Not listed

**Community Right-to-Know (Sections 311 and 312) :** Not Listed

## **Section 16. Additional information**

**Date of issue:** April 1<sup>st</sup>, 2024

**Version:** 4

**Elaborated by:** Toxyscan Inc., 1-866-780-0599

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*This safety data sheet has been prepared in accordance with the OSHA (USA), WHMIS (Canada) / GHS classification rules in effect at the time of writing.*