

## Hexanoic-4,4,5,5,6,6,6-d<sub>7</sub> Acid

### Section 1. Chemical product and company identifications

**Product code:** D-7331  
**Chemical formula:** C<sub>6</sub>H<sub>5</sub>D<sub>7</sub>O<sub>2</sub>  
**CAS:** 1276197-47-7  
**CAS (unlabelled):** 142-62-1  
**Synonyms:** *n*-Caproic Acid

**Supplier / Manufacturer:**

**C/D/N Isotopes Inc.**  
88 Leacock Street  
Pointe-Claire (Québec) H9R 1H1  
Phone: 514-697-6254  
Toll-Free (Canada & USA): 1-800-565-4696  
Fax: 514-697-6148  
Website: www.cdnisotopes.com

**In case of emergency:**

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

### Section 2. Hazards identifications

**Physical state:** Liquid

**Warning:** Harmful if swallowed or inhaled. Toxic in contact with skin. Causes severe skin burns and eye damage.


**Routes of entry:** Inhalation, ingestion, skin and eyes

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

**GHS Classification:**

- Acute toxicity, Oral (Category 4)
- Acute toxicity, Dermal (Category 3)
- Acute toxicity, Inhalation (Category 4)
- Skin corrosion (Category 1B)
- Serious eye damage (Category 1)

**GHS Label elements:**

- Pictograms: 
- Signal word: Danger

**Hazards statement:**

- H302 + H332 Harmful if swallowed or inhaled.
- H311 Toxic in contact with skin.
- H314 Causes severe skin burns and eye damage.

**Precautionary statement:**

- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P302 + P352 IF ON SKIN: Wash with plenty of soap and 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.
- P316 Get emergency medical help immediately.

### Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
Hexanoic-4,4,5,5,6,6,6-d <sub>7</sub> Acid	1276197-47-7	> 98

## **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.

## **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.

**Lower explosion limit:** 1.3 Vol%

**Upper explosion limit:** 9.3 Vol%

**Auto-ignition temperature:** 380 °C (716 °F)

**Flash point:** 102 °C (216 °F)

**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.

**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.

**Storage:** Store at room temperature. Adequate ventilation.

## **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:** 116.16 g/mol

**Physical status:** Liquid

**Color:** Colorless

**Odour:** Stench

**Density:** 0.927 g/cm<sup>3</sup>

**Melting point:** -4 °C (25 °F)

**Boiling point:** 202 - 203 °C (396 - 397 °F)

**Vapour pressure:** 0.24 hPa (0.18 mmHg) at 20 °C (68 °F)

**Vapour density:** 4.01 (Air = 1)

**Partition coefficient (octanol/water):** log Pow: 1.92

**Water solubility:** 10.3 g/L

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

**Stability and reactivity:** Stable under recommended storage conditions.

**Incompatibility:** Strong oxidizing agents.

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

**Reactivity conditions:** No data available.

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

**Toxicological data:** Hexanoic Acid

### **Information on ingredients:**

<b><u>Name</u></b>	<b><u>CAS</u></b>	<b><u>LD<sub>50</sub></u></b>	<b><u>LC<sub>50</sub></u></b>
Hexanoic Acid	142-62-1	Oral - Rat - 1,904 mg/kg Dermal - Rabbit - 584 mg/kg	Inhalation - Mouse - 2 h - 4,100 mg/m <sup>3</sup>

### **Potential acute effects**

- **Eyes:** Causes severe eye damage.
- **Skin:** Toxic if absorbed through skin. Causes severe skin burns.
- **Inhalation:** Harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Harmful if swallowed.

### **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><u>Name</u></b>	<b><u>Results</u></b>	<b><u>Species</u></b>	<b><u>Period</u></b>
Hexanoic Acid	88 mg/l LC50 22 mg/l EC50	Pimephales promelas Daphnia magna	96 h 24 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:** Aerobic. Result: 84 % - Readily biodegradable. Method: OECD Test guideline 301D.

**Bioaccumulative potential:** No data available.

## **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:** Caproic Acid

**UN number:** UN2829

**Class:** 8

**Packaging group:** III

**Additional information:** None

## Section 15. Regulatory information

### UNITED STATES: NFPA classification



Health: 3  
Flammable: 1  
Reactivity: 0  
Special conditions: None

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

### U.S. Federal regulations:

**TSCA 8(b) inventory:** Hexanoic Acid

**SARA 302/304/311/312 extremely hazardous substances:** Not Listed

**SARA 302/304 emergency planning and notification:** Not Listed

**SARA 302/304/311/312 hazardous chemicals:** Not Listed

**SARA 311/312 MSDS distribution - chemical inventory - hazard identification:** Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Listed

**CWA (Clean Water Act) 307:** Not Listed

**CWA (Clean Water Act) 311:** Not Listed

**CAA (Clean Air Act) 112 accidental release prevention:** Not Listed

**CAA (Clean Air Act) 112 regulated flammable substances:** Not Listed

**CAA (Clean Air Act) 112 regulated toxic substances:** Not Listed

### State regulations:

**DEA List I Chemicals (Precursor Chemicals):** Not Listed

**DEA List II Chemicals (Essential Chemicals):** Not Listed

**Substances in Massachusetts:** Listed

**Dangerous substances in New Jersey:** Listed

**New York – Dangerous substances with acute effects:** Not Listed

**Dangerous substances in Pennsylvania – right to know:** Listed

### WHMIS (Canada):



D1B - Toxic material causing immediate and serious toxic effects



D2B - Toxic material causing other toxic effects



E - Corrosive Material

## Section 16. Additional information

### References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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

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