Safety Data Sheet

Hexanoic-2,2-d_2 Acid

Section 1. Chemical product and company identifications

Product code: D-1231
Chemical formula: $C_6H_{10}D_2O_2$
CAS: 55320-65-5
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:

TOXYSCAN 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

Name	CAS	Concentration %
Hexanoic-2,2-d_2 Acid	55320-65-5	> 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^3
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:

Name	CAS	LD_{50}	LC_{50}
Hexanoic Acid	142-62-1	Oral - Rat - 1,904 mg/kg Dermal - Rabbit - 584 mg/kg	Inhalation - Mouse - 2 h - 4,100 mg/m^3

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:

Name	Results	Species	Period
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.

Date of issue: **May 28th, 2020**
Version: 3
Elaborated by: **Toxyscan Inc., 1-866-780-0599**
Notice to reader: To the best of our knowledge, the information contained herein is accurate. However, C/D/N Isotopes Inc., Toxyscan Inc., or any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.