



# Safety Data Sheet

## 1-Heptyne-6,6,7,7,7-d5

### Section 1. Chemical product and company identifications

**Product code:** D-6628

**Chemical formula:** C<sub>7</sub>H<sub>7</sub>D<sub>5</sub>

**CAS:** 83418-35-3

**CAS (unlabelled):** 628-71-7

**Synonyms:** Amylacetylene

#### 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](http://www.cdnisotopes.com)

#### In case of emergency:

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

### Section 2. Hazards identifications

**Physical state:** Liquid

**Warning:** Highly flammable liquid and vapour. Causes skin irritation. Causes serious eye irritation.

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

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

##### GHS Classification:

- Flammable liquids (Category 2)
- Skin irritation (Category 2)
- Eye irritation (Category 2A)
- Specific target organ toxicity - single exposure (Category 3)
- Aspiration hazard (Category 1)

##### GHS Label elements:

- Pictograms:   
- Signal word: Danger

##### Hazards statement:

- H225 Highly flammable liquid and vapour.
- H304 May be fatal if swallowed and enters airways.
- H315 Causes skin irritation.
- 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.
- 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 + P350 IF ON SKIN: Wash with plenty of soap and water.
- 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>
1-Heptyne-6,6,7,7,7-d <sub>5</sub>	83418-35-3	> 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. Keep away from heat/sparks/open flame/hot surface. No smoking.

**Lower explosion limit:** No data available

**Upper explosion limit:** No data available

**Auto-ignition temperature:** No data available

**Flash point:** -2 °C (28 °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. Remove all sources of ignition.

**Environmental precautions:** Do not let product enter drains.

**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 at room temperature. Adequate ventilation. Protect from heat and ignition sources.

## **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) or CEN (EU).

**Hands:** 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.

**Skin/body:** 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.

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

**Molecular weight:** 96.17 g/mol

**Physical status:** Liquid

**Color:** Colorless to yellow

**Odour:** No data available

**Density:** 0.733 g/cm<sup>3</sup>

**Melting point:** -81 °C (-114 °F)

**Boiling point:** 99 - 100 °C (210 - 212 °F)

**Vapour pressure:** 70 hPa (52.5 mmHg) at 25 °C (77 °F)

**Vapour density:** No data available

**Partition coefficient (octanol/water):** No data available

**Water solubility:** 94 mg/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:** Heat, flames and sparks.

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

**Toxicological data:** 1-Heptyne

**Information on ingredients:**

<u>Name</u>	<u>CAS</u>	<u>LD<sub>50</sub></u>	<u>LC<sub>50</sub></u>
1-Heptyne	628-71-7	No data available	No data available

### **Potential acute effects**

- **Eyes:** Causes serious eye irritation.
- **Skin:** May be harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** May be harmful if swallowed. Aspiration hazard if swallowed - can enter lungs and cause damage.

### **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:**

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
1-Heptyne	No data available		

**Effects on environment:** No data available

**Mobility:** No data available

**Environmental precautions:** No data available

**Persistence and degradability:** No data available

**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:** Flammable liquid, n.o.s. (1-Heptyne)

**UN number:** UN1993

**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:

TSCA 8(b) inventory: 1-Heptyne

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: Not 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: Not Listed

Dangerous substances in New Jersey: Not Listed

New York – Dangerous substances with acute effects: Not Listed

Dangerous substances in Pennsylvania – right to know: Not Listed

### WHMIS (Canada):



B2 - Flammable liquid



D2B - Toxic material causing other toxic effects

## 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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