



## *n*-Hexyl-5,5,6,6,6-d<sub>5</sub> Alcohol

### **Section 1. Chemical product and company identifications**

**Product code:** D-6960  
**Chemical formula:** C<sub>6</sub>H<sub>9</sub>D<sub>5</sub>O  
**CAS:** 64118-18-9  
**CAS (unlabelled):** 111-27-3  
**Synonyms:** 1-Hexanol

**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:** Flammable liquid and vapour. Harmful if swallowed or in contact with skin. Causes serious eye irritation.



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

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

**GHS Classification:**

- Flammable liquids (Category 3)
- Acute toxicity, Oral (Category 4)
- Acute toxicity, Dermal (Category 4)
- Skin irritation (Category 3)
- Eye irritation (Category 2A)

**GHS Label elements:**

- Pictograms:  
- Signal word: Danger

**Hazards statement:**

- H226 Flammable liquid and vapour.
- H302 + H312 Harmful if swallowed or in contact with skin
- H316 Causes mild skin irritation.
- H319 Causes serious eye irritation.

**Precautionary statement:**

- P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.
- P280 Wear protective gloves/ protective clothing.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
<i>n</i> -Hexyl-5,5,6,6,6-d <sub>5</sub> Alcohol	64118-18-9	> 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:** Do NOT induce vomiting. 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:** 1.2 Vol%

**Upper explosion limit:** 7.7 Vol%

**Auto-ignition temperature:** 292 °C (558 °F)

**Flash point:** 60 °C (140 °F) - closed cup

**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. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

**Environmental precautions:** Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up:** Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

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

**Handling:** Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build-up of electrostatic charge.

**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:** Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as 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:** 102.18 g/mol

**Physical status:** Liquid

**Color:** Colourless

**Odour:** Sweet

**Density:** 0.814 g/mL at 25 °C (77 °F)

**Melting point:** -52 °C (-62 °F) - lit.

**Boiling point:** 156 - 157 °C (313 - 315 °F) - lit.

**Vapour pressure:** 1hPa (0.75 mmHg) at 20 °C (68 °F)

**Vapour density:** 3.53 (Air = 1)

**Partition Coefficient (octanol/water):** log Pow: 2.03

**Water solubility:** 5.9 g/L

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

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

**Incompatibility:** Strong oxidizing agents, strong acids.

**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-Hexanol

**Information on ingredients:**

<b>Name</b>	<b>CAS</b>	<b>LD<sub>50</sub></b>	<b>LC<sub>50</sub></b>
1-Hexanol	111-27-3	Oral - rat - 720 mg/kg	No data available

### **Potential acute effects**

- **Eyes:** Causes eye irritation.
- **Skin:** Harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. Causes 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:** Genotoxicity in vitro - Not mutagenic in Ames Test. Histidine reversion (Ames).
- **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>
1-Hexanol	97.7 mg/l LC50 > 100 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:** > 70 % - Readily biodegradable.

**Bioaccumulative potential:** Oncorhynchus mykiss (rainbow trout) - 24 h. Bioconcentration factor (BCF): 0.5.

## **Section 13. Disposal considerations**

**Waste disposal:** Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

## **Section 14. Transportation information**

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

**Shipping name:** Hexanols

**UN number:** UN2282

**Class:** 3

**Packaging group:** III

**Additional information:** None

## **Section 15. Regulatory information**

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



Health: 2  
Flammable: 2  
Reactivity: 0  
Specials conditions: None

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

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

**TSCA 8(b) inventory:** 1-Hexanol

**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:** Not 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):**



B3 - Combustible 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.

**Date of issue:** March 1st, 2017

**Version:** 1

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

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