



# 2-Methyl-d<sub>3</sub>-3-butyn-1,1,1-d<sub>3</sub>-2-ol

### Section 1. Chemical product and company identifications

Product code: D-6586 Chemical formula: C<sub>5</sub>H<sub>2</sub>D<sub>6</sub>O CAS: 57444-27-6 CAS (unlabelled): 115-19-5 Synonyms: 1,1-Dimethylpropargyl Alcohol

#### Supplier / Manufacturer:

# C/D/N Isotopes Inc.

In case of emergency: **TOXYSCAN HOTLINE: 1-855-780-0599** 

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

# Section 2. Hazards identifications

Physical state: Liquid

Warning: Highly flammable liquid and vapour. Harmful if swallowed. Causes serious eye damage. Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:	<ul> <li>Flammable liquids (Category 2)</li> <li>Acute toxicity, Oral (Category 4)</li> <li>Serious eye damage (Category 1)</li> </ul>
GHS Label elements:	- Pictograms:
	- Signal word: Danger
Hazards statement:	- H225 Highly flammable liquid and vapour. - H302 Harmful if swallowed. - H318 Causes serious eye damage.
Precautionary statement:	<ul> <li>P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.</li> <li>P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.</li> <li>P301 + P 330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.</li> <li>P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.</li> <li>P317 Get medical help.</li> </ul>

### Section 3. Composition and information on ingredients

Name	<u>CAS</u>	Concentration %
2-Methyl-d <sub>3</sub> -3-butyn-1,1,1-d <sub>3</sub> -2-ol	57444-27-6	> 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: 1.8 Vol%
Upper explosion limit: 16 Vol%
Auto-ignition temperature: 350 °C (662 °F)
Flash point: 20 °C (68 °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).

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: 84.12 g/mol Physical status: Liquid Color: Colorless Odour: No data available Density: 0.868 g/mL Melting point: 3 °C (37 °F) Boiling point: 104 °C (219 °F) Vapour pressure: 20 hPa (15 mmHg) at 20 °C (68 °F) Vapour density: 2.9 (Air = 1) Partition coefficient (octanol/water): log Pow: 0.28 Water solubility: Soluble

### Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
 Incompatibility: Strong oxidizing agents, acids, copper.
 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: 2-Methyl-3-butyn-2-ol

### Information on ingredients:

<u>Name</u>	CAS	

2-Methyl-3-butyn-2-ol 115-19-5 Oral - Rat - 1,950 mg/kg

LC<sub>50</sub> No data available

**Potential acute effects** 

- Eyes: Causes serious eye damage.
- Skin: May be harmful if absorbed through skin. May cause skin irritation.
- Inhalation: May be harmful if inhaled. May cause respiratory tract irritation.

LD50

- 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 Ames test S. typhimurium with and without metabolic activation negative. Genotoxicity in vivo - Mouse - male and female - Intraperitoneal - negative.
- 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>
2-Methyl-3-butyn-2-ol	3,400 mg/l LC50 > 500 mg/l EC50 > 500 mg/l EC50	Leuciscus idus Daphnia magna Desmodesmus subspicatus	96 h 48 h 72 h

Effects on environment: No data available. Mobility: No data available. Environmental precautions: No data available. Persistence and degradability: Not readily biodegradable. 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: Alcohols, n.o.s. (2-Methylbutynol) UN number: UN1987 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: 2-Methyl-3-butyn-2-ol 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: 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):

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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