

2-Octanone-1,1,1,3,3-d₅

Section 1. Chemical product and company identifications

Product code: D-8349

Chemical formula: C₈D₅H₁₁O

CAS: 17827-52-0

CAS (unlabelled): 111-13-7

Synonyms: Octan-2-one; Hexyl methyl ketone; 2-Oxooctane

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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Section 2. Hazards identifications

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

GHS Classification:

- Flammable liquids (Category 3)
- Acute toxicity, Dermal (Category 4)

GHS Label elements:

- Pictograms:  
- Signal word: Warning

Hazards statement:

- H226 Flammable liquid and vapour.
- H312 Harmful in contact with skin

Precautionary statement:

- P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.
- P233 Keep container tightly closed.
- P240 Ground/bond container and receiving equipment.
- P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
- P242 Use non-sparking tools.
- P243 Take action to prevent static discharges.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P302 + P352 IF ON SKIN: wash with plenty of soap and water.
- P303 + P361 + P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
- P362 + P364 Take off contaminated clothing and wash it before reuse.
- P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
- P501 Dispose of contents/ container to an approved waste disposal plant.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
2-Octanone-1,1,1,3,3,3-ds	17827-52-0	> 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.

Indication of immediate medical attention and special treatment needed, if necessary: No data available.

Most important symptoms and effects, both acute and delayed: Redness, skin irritation.

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.

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. 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. Keep away from sources of ignition - No smoking.

Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources. Protect from light.

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: 128.21 g/mol
Physical status: Liquid
Color: Colorless
Odour: No data available
Density: 0.819 g/cm³
Melting point: -16 °C (3 °F)
Boiling point: 173 °C (343 °F)
Vapour pressure: No data available
Vapour density: No data available
Partition coefficient (octanol/water): No data available
Water solubility: No data available
Lower explosion limit: No data available
Upper explosion limit: No data available
Auto-ignition temperature: No data available
Flash point: 56 °C (133 °F)

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: 2-Octanone

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
2-Octanone	111-13-7	Intraperitoneal - Rat - 800 mg/kg Oral - Rat - 3,089 mg/kg Skin - Rabbit - 1,337 mg/kg	Inhalation - Rat - 6H - > 2,136 ppm

Potential acute effects

- **Eyes:** No data available.
- **Skin:** Harmful in contact with skin.
- **Inhalation:** No data available.
- **Ingestion:** No data available.

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>
2-Octanone	36 mg/l LC50	Pimephales promelas	96h

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: 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: Ketones, liquid, n.o.s. (2-Octanone)

UN number: UN1224

Class: 3

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 1
Flammable: 2
Reactivity: 0
Special conditions: None

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

U.S. Federal regulations:

California proposition 65 requirements : Not listed

SARA section 313 (specific toxic chemical listings) : Not listed

CERCLA reportable quantity : Not listed

Sections 302-304 reportable quantity : Not listed

Community Right-to-Know (Sections 311 and 312) : Not Listed

Section 16. Additional information

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

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This safety data sheet has been prepared in accordance with the OSHA (USA), WHMIS (Canada) / GHS classification rules in effect at the time of writing.