

3-Methyl-2-Butanone-1,1,1,3-d₄

Section 1. Chemical product and company identifications

Product code: D-8390

Chemical formula: C₅H₈D₄O

CAS: 31599-94-7

CAS (unlabelled): 563-80-4

Synonyms: Isopropyl methyl ketone

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

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

GHS Classification: - Flammable liquids (Category 2)
- Specific target organ toxicity - single exposure (Category 3), Central nervous system

GHS Label elements: - Pictograms:  
- Signal word: Danger

Hazards statement: - H225 Highly flammable liquid and vapour.
- H336 May cause drowsiness or dizziness.

Precautionary statement: - P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.
- P233 Keep container tightly closed.
- P240 Ground and 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.
- P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
- P271 Use only outdoors or in a well-ventilated area.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
- P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P403 + P235 Store in a well-ventilated place. Keep cool.
- P405 Store locked up.
- 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>
3-Methyl-2-Butanone-1,1,1,3-d ₄	31599-94-7	> 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: No data available.

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.

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: 86.13 g/mol

Physical status: Liquid

Color: Colorless

Odour: No data available

Density: 0.805 g/cm³

Melting point: No data available

Boiling point: 93 - 95 °C (199 - 203 °F)

Vapour pressure: 70 hPa (53 mmHg) at 25 °C (77 °F)

Vapour density: 2.90 (Air = 1)

Partition coefficient (water): log Pow: 2.29

Water solubility: 8.21 g/l

Lower explosion limit: 1.5 Vol%

Upper explosion limit: 8.2 Vol%

Auto-ignition temperature: 448 °C (838 °F) at 980 hPa (735 mmHg)

Flash point: -3 °C (27 °F)

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing/ reducing agents, strong bases.

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: 3-Methyl-2-Butanone

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
3-Methyl-2-Butanone	563-80-4	Oral - Rat – 3,078 mg/kg Dermal - Rabbit - 6,350 mg/kg	Inhalation - Rat - 6 h – 34,250 mg/m ³

Potential acute effects

- **Eyes:** No data available.
- **Skin:** No data available.
- **Inhalation:** May cause drowsiness or dizziness if inhaled.
- **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:** In vitro mammalian cell gene mutation test - with and without metabolic activation – negative, Ames test - Escherichia coli/Salmonella typhimurium - with and without metabolic activation - 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>
3-Methyl-2-Butanone	68 mg/l LC50	Oncorhynchus mykiss	96 h
	81 mg/l EC50	Daphnia magna	48 h
	44.23 mg/l EC50	Pseudokirchneriella subcapitata	72 h

Effects on environment: No data available.

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: 3-Methylbutan-2-one

UN number: UN2397

Class: 3

Packaging group: II

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 1
Flammable: 3
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.