

4-(N-Methyl-N-nitrosoamino)-1-(3-pyridyl-d₄)-1-butanone

Section 1. Chemical product and company identifications

Product code: D-4152

Chemical formula: C₁₀H₉D₄N₃O₂

CAS: 764661-24-7

CAS (unlabelled): 64091-91-4

Synonyms: 4-(Methylnitrosoamino)-1-(3-pyridinyl)-1-butanone, 4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone, NNK

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

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

GHS Classification:

- Acute toxicity, Oral (Category 3)
- Skin sensitisation (Category 1)
- Carcinogenicity (Category 1A)

GHS Label elements:

- Pictograms:   
- Signal word: Danger

Hazards statement:

- H301 Toxic if swallowed.
- H317 May cause an allergic skin reaction.
- H350 May cause cancer.

Precautionary statement:

- P202 Do not handle until all safety precautions have been read and understood.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
- P264 Wash hands thoroughly after handling.
- P270 Do not eat, drink or smoke when using this product.
- P272 Contaminated work clothing should not be allowed out of the workplace.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
- P316 Get emergency medical help immediately.
- P330 Rinse mouth
- P333 +P313 If skin irritation or rash occurs: Get medical advice/ attention.
- P362 +P364 Take off immediately all contaminated clothing and wash it before reuse.
- 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>
4-(N-Methyl-N-nitrosoamino)-1-(3-pyridyl-d ₄)-1-butanone	764661-24-7	> 98

Section 4. First aid measures

Eye contact: Flush eyes with water as a precaution.

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: Not flammable or combustible.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, nitrogen 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 dust formation. Ensure adequate ventilation. Avoid breathing dust.

Environmental precautions: Do not let product enter drains.

Methods for cleaning up: Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation.

Storage: Store at room temperature. Adequate ventilation.

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: 207.23 g/mol

Physical status: Solid

Color: White to yellowish

Odour: No data available

Density: No data available

Melting point: 64 - 66 °C (147 - 151 °F)

Boiling point: No data available

Vapour pressure: No data available

Vapour density: No data available

Partition coefficient (octanol/water): Log Pow:0.53

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: No data available

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, nitrogen oxides.

Reactivity conditions: No data available.

Section 11. Toxicological information (unlabelled)

Toxicological data: 4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone	64091-91-4	Intraperitoneal - Mouse - 1,000 mg/kg	No data available

Potential acute effects

- **Eyes:** No data available.
- **Skin:** May cause an allergic skin reaction.
- **Inhalation:** No data available.
- **Ingestion:** Toxic if swallowed.

Potential acute effects

- **Carcinogenic effects:** Carcinogenicity - Hamster - Subcutaneous. Tumorigenic: Carcinogenic by RTECS criteria. Sense Organs and Special Senses (Nose, Eye, Ear, and Taste): Olfaction: Tumors. Lungs, Thorax, or Respiration: Tumors. This product is or contains a component that has been reported to be probably carcinogenic based on its IARC, OSHA, ACGIH, NTP, or EPA classification. Limited evidence of carcinogenicity in animal studies. IARC: 1 - Group 1: Carcinogenic to humans (4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone). 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 - rabbit - Other cell types. DNA damage. Genotoxicity in vivo - rat - Intraperitoneal. Micronucleus test
- **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>
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone	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:

DOT (Shipping name): Toxic solid, organic, n.o.s. [4-(N-Methylnitrosoamino)-1-(3-pyridyl)-1-butanone]

UN number: UN2811

Class: 6.1

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 2
Flammable: 0
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

Date of issue: February 10th, 2023

Version: 4

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

Notice to reader: To the best of our knowledge, the information contained herein is accurate. However, C/D/N Isotopes Inc., Toxyscan Inc., or any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

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.