



# Safety Data Sheet - Version 5.0

Preparation Date 10/4/2013

Latest Revision Date (If Revised) 1/10/2017

SDS Expiry Date 1/9/2020

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1 Product Identifier

**Chemical Name** 4-(Methylnitrosamino)-1-(3-pyridyl-d4)-1-butanone (0.1 mg/mL in Methanol)

**Catalogue #** KIT0770

### 1.2 Relevant Identified Uses of the Substance or Mixture and Uses Advised Against

**Product Uses** To be used only for scientific research and development. Not for use in humans or animals.

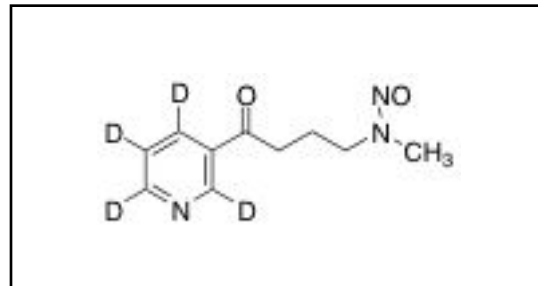
### 1.3 Details of the Supplier of the Safety Data Sheet

**Company** Toronto Research Chemicals  
2 Brisbane Road  
Toronto, ON M3J 2J8  
CANADA

**Telephone** +14166659696

**FAX** +14166654439

**Email** orders@trc-canada.com



### 1.4 Emergency Telephone Number

**Emergency#** +14166659696 between 0800-1700 (GMT-5)

## 2. HAZARDS IDENTIFICATION

### WHMIS Classification (Canada)

B2 Flammable Liquid

D1A Very Toxic Material Causing Immediate and Serious Toxic Effects  
Toxic by Inhalation/Skin Absorption/Inhalation

D2B Toxic Material Causing Other Toxic Effects  
Moderate Skin/Eye Irritant

### WHMIS Symbols (Canada)



### 2.1/2.2 Classification of the Substance or Mixture and Label Elements

#### GHS Hazards Classification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Flammable Liquids (Category 2)

Acute Toxicity, Dermal (Category 3)

Acute Toxicity, Inhalation (Category 3)

Acute Toxicity, Oral (Category 3)

Serious Eye Irritation (Category 2A)

Skin Irritation (Category 2)

#### EU Classification (According to EU Regulation 67/548/EEC)

Highly flammable. Toxic by inhalation, in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin.

#### EU Risk and Safety Statements (According to EU Regulation 67/548/EEC)

##### Hazard Statements

Highly Flammable

Toxic

Irritant

##### Hazard Codes

F

T

Xi



### Risk Codes and Phrases

- R11 Highly flammable.  
R23/24/25 Toxic by inhalation, in contact with skin and if swallowed.  
R36/37/38 Irritating to eyes, respiratory system and skin.

### Safety Precaution Codes and Phrases

- S15 Keep away from heat.  
S36/37/39 Wear suitable protective clothing, gloves and eye/face protection.  
S46 If swallowed, seek medical advice immediately and show this container or label.  
S27/28 After contact with skin, take off immediately all contaminated clothing and wash with plenty of soap and water.

### GHS Hazards Identification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

Signal Word Danger



### GHS Hazard Statements

- H225 Highly flammable liquid and vapour.  
H311 Toxic in contact with skin.  
H331 Toxic if inhaled.  
H301 Toxic if swallowed.  
H319 Causes serious eye irritation.  
H315 Causes skin irritation.

### GHS Precautionary Statements

- P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P210 Keep away from heat/sparks/open flames/hot surfaces. – No smoking.  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray  
P301/P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
P305/P351/P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P303/P361/P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.

### 2.3 Unclassified Hazards/Hazards Not Otherwise Classified

No data available.

## **3. COMPOSITION/INFORMATION ON INGREDIENTS**

### 3.1 Substances

Molecular Formula: C<sub>10</sub>H<sub>9</sub>D<sub>4</sub>N<sub>3</sub>O<sub>2</sub>

Molecular Weight: 211.25

CAS Registry #: 764661-24-7

EC#:

### Synonyms

4-(N-Methyl-N-nitrosamino)-1-(3-pyridyl-d4)-1-butanone; NNK-d4;

### 3.2 Mixtures

<u>Ingredient</u>	<u>CAS#</u>	<u>EC#</u>	<u>Index-No.</u>	<u>%Composition</u>
4-(Methylnitrosamino)-1-(3-pyridyl-d4)-1-butanone	764661-24-7	N/A	N/A	0.013%
Methanol	67-56-1	200-659-6	603-001-00-X	>99.9%

## **4. FIRST AID MEASURES**

### 4.1 Description of First Aid Measures

#### General Advice

If medical attention is required, show this safety data sheet to the doctor.

#### If Inhaled

If inhaled, move casualty to fresh air. If not breathing, give artificial respiration and consult a physician.

### **In Case of Skin Contact**

Remove contaminated clothing and shoes. Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

### **In Case of Eye Contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

### **If Swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Center. Seek medical attention.

### **4.2 Most Important Symptoms and Effects, Both Acute and Delayed**

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or section 11.

### **4.3 Indication of any Immediate Medical Attention and Special Treatment Needed**

No data available.

## **5. FIREFIGHTING MEASURES**

### **5.1 Extinguishing Media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### **5.2 Special Hazards Arising from the Substance or Mixture**

Carbon oxides, Nitrogen oxides

### **5.3 Advice for Firefighters**

Wear self contained breathing apparatus for fire fighting if necessary.

### **5.4 Further Information**

No data available.

## **6. ACCIDENTAL RELEASE MEASURES**

### **6.1 Personal Precautions, Protective Equipment and Emergency Procedures**

Use recommended personal protective equipment (see Section 8). Adequate ventilation must be provided to ensure vapours or mists are not inhaled. Vapours are heavier than air and may accumulate in low areas. All sources of ignition, including sources of static discharge, must be removed from area.

### **6.2 Environmental Precautions**

Material should not be allowed to enter the environment. Prevent further spillage or discharge into drains, if safe to do so.

### **6.3 Methods and Materials for Containment and Cleaning Up**

Contain the spill and then collect using non-combustible absorbent material (such as clay, diatomaceous earth, vermiculite or other appropriate material). Place material in a suitable, sealable container and then dispose according to local/national regulations and guidance (see Section 13).

### **6.4 Reference to Other Sections**

For protective equipment, refer to Section 8. For disposal, see Section 13.

## **7. HANDLING AND STORAGE**

### **7.1 Precautions for Safe Handling**

Avoid contact with skin and eyes. Ventilation and proper handling are to be used to prevent the formation of vapours and mists. Remove all sources of ignition and take precautionary measures to prevent the buildup of electrostatic discharge (ground and bond containers as appropriate). No smoking, eating or drinking around this material. Wash hands after use.

### **7.2 Conditions for Safe Storage, Including any Incompatibilities**

Ensure container is kept securely closed before and after use. Keep in a well ventilated area and do not store with strong oxidizers or other incompatible materials (see Section 10).

Storage conditions: Amber Vial, -20°C Freezer, Under inert atmosphere

### **7.3 Specific End Uses**

For scientific research and development only. Not for use in humans or animals.

## **8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

## 8.1 Control Parameters

### Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200.000000 ppm 262.000000 mg/m3	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)

### Remarks

Substance may be readily absorbed through intact skin

STEL	250.000000 ppm 328.000000 mg/m3	Canada. Alberta, Occupational Health and Safety Code (table 2: OEL)
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Substance may be readily absorbed through intact skin

TWA	200.000000 ppm	Canada. British Columbia OEL
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Contributes significantly to the overall exposure by the skin route.

STEL	250.000000 ppm	Canada. British Columbia OEL
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Contributes significantly to the overall exposure by the skin route.

TWAEV	200.000000 ppm 262.000000 mg/m3	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
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Skin (percutaneous)

STEV	250.000000 ppm 328.000000 mg/m3	Québec. Regulation respecting occupational health and safety, Schedule 1, Part 1: Permissible exposure values for airborne contaminants
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Skin (percutaneous) 200.000000 ppm USA. ACGIH Threshold Limit Values (TLV)

STEL	250.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
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## 8.2 Exposure Controls

### Appropriate Engineering Controls

A laboratory fumehood or other appropriate form of local exhaust ventilation should be used to avoid exposure.

### Personal Protective Equipment

All recommendations below are advisory in nature and a risk assessment should be performed by the employer/end user prior to use of this product. The type of protective equipment must be selected based on the amount and concentration of the dangerous material being used in the workplace.

### Eye/Face Protection

Safety goggles or face shield. All equipment should have been tested and approved under appropriate standards, such as NIOSH (US), CSA (Canada), or EN 166 (EU).

### Skin Protection

Gloves should be used when handling this material. Gloves are to be inspected prior to use. Contaminated gloves are to be removed using proper glove removal technique so that the outer surface of the glove does not contact bare skin. Dispose of contaminated gloves after use in compliance with good laboratory practices and local requirements.

Gloves used for incidental exposures (splash protection) should be designated as "chemical resistant" by EU standard EN 374 with the resistance codes corresponding to the anticipated use of the material. Unrated gloves are not recommended.

Suggested gloves: AnsellPro Sol-Vex nitrile gloves style 37-175, 15 mil thickness.  
Penetration time has not been determined.

Gloves used for prolonged direct exposure (immersion) should be designated "chemical resistant" as per EN 734 with the resistance codes corresponding to the anticipated use of the material.

Suggested gloves: AnsellPro Viton/Butyl gloves style 38-612, 4/8 mil thickness.  
Penetration time has not been determined.

These recommendations may not apply if the material is mixed with any other chemical, or dissolved into a solution. A risk assessment must be performed to ensure the gloves will still offer acceptable protection.

### Body Protection

Fire resistant (Nomex) coveralls or chemical-resistant bodysuit (laminated Tychem SL or equivalent).

### Respiratory Protection

Recommended respirators are NIOSH-approved N100 or CEN-approved FFP3 particulate respirators. These are to be only used as a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator must be used.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on Basic Physical and Chemical Properties

#### A) Appearance

Clear Colourless Solution

#### C) Odour Threshold

No data available

#### E) Melting Point/Freezing Point

N/A

#### G) Flash point

No data available

#### I) Flammability (Solid/Gas)

No data available

#### K) Vapour Pressure

No data available

#### M) Relative Density

No data available

#### O) Partition Coefficient: n-octanol/water

No data available

#### Q) Decomposition Temperature

No data available

#### S) Explosive Properties

No data available

#### B) Odour

No data available

#### D) pH

No data available

#### F) Initial Boiling Point/Boiling Range

No data available

#### H) Evaporation Rate

No data available

#### J) Upper/Lower Flammability/Explosive Limits

No data available

#### L) Vapour Density

No data available

#### N) Solubility

Methanol

#### P) Auto-Ignition Temperature

No data available

#### R) Viscosity

No data available

#### T) Oxidizing Properties

No data available

### 9.2 Other Information

no data available

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available.

### 10.2 Chemical Stability

Stable under recommended storage conditions.

### 10.3 Possibility of Hazardous Reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to Avoid

Heat, flames sparks. Extremes of temperature and direct sunlight.

### 10.5 Incompatible Materials

Acid chlorides, Acid anhydrides, Oxidizing agents, Alkali metals, Reducing Agents, Acids.

### 10.6 Hazardous Decomposition Products

In the event of fire: See section 5. Other decomposition products: No data available.

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on Toxicological Effects

#### A) Acute Toxicity

Oral LD50: No data available.

Inhalation LC50: No data available.

Dermal LD50: No data available.

**B) Skin Corrosion/Irritation**

No data available

**C) Serious Eye Damage/Irritation**

No data available

**D) Respiratory or Skin Sensitization**

No data available

**E) Germ Cell Mutagenicity**

No data available

**F) Carcinogenicity**

No data available

**G) Reproductive Toxicity/Teratogenicity**

No data available

**H) Single Target Organ Toxicity - Single Exposure**

No data available

**I) Single Target Organ Toxicity - Repeated Exposure**

No data available

**J) Aspiration Hazard**

No data available

**K) Potential Health Effects and Routes of Exposure**

**Inhalation**

Toxic if inhaled. Causes respiratory tract irritation.

**Ingestion**

Toxic if swallowed.

**Skin**

Toxic if absorbed through skin. Causes skin irritation.

**Eyes**

Causes eye irritation.

**L) Signs and Symptoms of Exposure**

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or section 11.

To the best of our knowledge, the chemical, physical, and toxicological properties of this material have not been thoroughly investigated.

**M) Additional Information**

RTECS: PC1400000 (Methanol)

**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**

No data available.

**12.2 Persistence and Degradability**

No data available.

**12.3 Bioaccumulative Potential**

No data available.

**12.4 Mobility in Soil**

No data available.

**12.5 Results of PBT and vPvB Assessment**

No data available.

**12.6 Other Adverse Effects**

No data available.

**13. DISPOSAL CONSIDERATIONS**

**13.1 Waste Treatment Methods**

**A) Product**

Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

**B) Contaminated Packaging**

Dispose of as above.

### C) Other Considerations

Product is not to be disposed of in sanitary sewers, storm sewers, or landfills.

## 14. TRANSPORT INFORMATION

### 14.1 UN Number

DOT (US): UN1230                      IATA: UN1230                      IMDG: UN1230                      ADR/RID: UN1230

### 14.2 UN Proper Shipping Name

DOT (US)/IATA:  
Methanol, solution  
IMDG/ARD/RID:  
METHANOL, SOLUTION

### 14.3 Transport Hazard Class(es)

DOT (US): 3                      IATA: 3                      IMDG: 3                      ADR/RID: 3

### 14.4 Packing Group

DOT (US): II                      IATA: II                      IMDG: II                      ADR/RID: II

### 14.5 Environmental Hazards

DOT (US): None                      IATA: None                      IMDG: None                      ADR/RID: None

### 14.6 Special Precautions for User

None

## 15. REGULATORY INFORMATION

This safety data sheet complies with the requirements of WHMIS (Canada), OSHA 1910.1200 (US), and EU Regulation EC No. 1907/2006 (European Union).

### 15.1 Safety, Health and Environmental Regulations/Legislation Specific for the Substance or Mixture

#### A) Canada

**DSL/NDSL Status:** This product or a component of this product is registered on the Canadian DSL/NDSL.

#### B) United States

**TSCA Status:** This product or a component is listed on the US EPA TSCA.

#### C) European Union

**ECHA Status:** This product or a component is registered with the EU ECHA.

### 15.2 Chemical Safety Assessment

No data available

## 16. OTHER INFORMATION

### 16.1 Revision History

Original Publication Date: 10/4/2013

### 16.2 List of Abbreviations

LD50	Median lethal dose of a substance required to kill 50% of a test population.
LC50	Medial lethal concentration of a substance required to kill 50% of a test population.
LDLo	Lowest known lethal dose
TDLo	Lowest known toxic dose
IARC	International Agency for Research on Cancer
NTP	National Toxicology Program
RTECS	Registry of Toxic Effects of Chemical Substances

### 16.3 Further Information

Copyright 2015. Toronto Research Chemicals Inc. Copies may be made for internal use only. The above information is believed to be correct to the best of our knowledge, but is to be only used as a guide. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Please take all due care when handling this product.