SAFETY DATA SHEET

Version 6.2
Revision Date 05/07/2021
Print Date 06/18/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) solution

Product Number : N-076
Brand : Cerilliant

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin sensitization (Category 1), H317
Carcinogenicity (Category 2), H351
Specific target organ toxicity - single exposure (Category 1), H370

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



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Signal word	Danger
Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H317	May cause an allergic skin reaction.
H351	Suspected of causing cancer.
H370	Causes damage to organs.
Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P361	Remove/ Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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.

Sensitizing components:
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone
May produce an allergic reaction.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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SECTION 3: Composition/information on ingredients

3.2 Mixtures

Molecular weight : 207.23 g/mol

Component		Classification	Concentration
Methanol			
CAS-No. EC-No. Index-No. Registration number	67-56-1 200-659-6 603-001-00-X 01-2119433307-44-XXXX	Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370 Concentration limits: >= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371;	>= 90 - <= 100 %
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone			
CAS-No.	64091-91-4	Acute Tox. 3; Skin Sens. 1; Carc. 2; H301, H317, H351	>= 0.1 - < 1 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Consult a physician. Show this material safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

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SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable 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

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion
Use explosion-proof equipment.**Advice on protection against fire and explosion**
Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

Hygiene measures
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage stability
Recommended storage temperature
-20 °C

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		TWA	200 ppm 260 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		ST	250 ppm 325 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	250 ppm 325 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		TWA	200 ppm 260 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

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		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methanol	67-56-1	Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 30 min
Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

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Respiratory protection
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) or CEN (EU).

Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	64 - 65 °C 147 - 149 °F at 1.013 hPa
g)	Flash point	9.7 °C (49.5 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 36 %(V) Lower explosion limit: 6 %(V)
k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information
No data available

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SECTION 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

Vapors may form explosive mixture with air.

10.4 Conditions to avoid
Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials
Acids, Oxidizing agents, Alkali metals, Strong oxidizing agents, Strong acids, Acid chlorides, Acid anhydrides, Reducing agents, Strong reducing agents, Phosphorus halides

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity
Oral: No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC: 1 - Group 1: Carcinogenic to humans (4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone)

IARC: 1 - Group 1: Carcinogenic to humans (4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone)

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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NTP: RAHC - Reasonably anticipated to be a human carcinogen (4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone)

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

Methyl alcohol may be fatal or cause blindness if swallowed., Cannot be made non-poisonous., Effects due to ingestion may include:, Nausea, Headache, Vomiting, Gastrointestinal disturbance, Dizziness, Weakness, Confusion.
Central nervous system - Breathing difficulties - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

Components

Methanol

Acute toxicity
Acute toxicity estimate Oral - 100.1 mg/kg
(Expert judgment)
Symptoms: Nausea, Vomiting
Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l
(Expert judgment)
Symptoms: Irritation symptoms in the respiratory tract.
Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgment)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
Remarks: (ECHA)
Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA)

Respiratory or skin sensitization
Sensitisation test: - Guinea pig

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Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Based on available data the classification criteria are not met.
Ames test
Salmonella typhimurium
Result: negative
In vitro mammalian cell gene mutation test
Chinese hamster lung cells
Result: negative
OECD Test Guideline 474
Mouse - male and female - Bone marrow
Result: negative

Carcinogenicity
Did not show carcinogenic effects in animal experiments.

Reproductive toxicity
Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure
Causes damage to organs. - Eyes, Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute oral toxicity - Nausea, Vomiting
Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone

Acute toxicity
LD50 Oral - 100 mg/kg
Inhalation: No data available
Dermal: No data available
LD50 Intraperitoneal - Mouse - 1,000 mg/kg

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitization
The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

Germ cell mutagenicity
Rabbit
Other cell types
Remarks: DNA damage

Rat
Remarks: Micronucleus test

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Carcinogenicity
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

Reproductive toxicity
No data available
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture
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
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

Components

Methanol

Toxicity to fish	flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

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4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

DOT (US)
UN number: 1230 Class: 3 Packing group: II
Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOLSOLUTION

IATA
UN number: 1230 Class: 3 (6.1) Packing group: II
Proper shipping name: MethanolSOLUTION

SECTION 15: Regulatory information

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

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Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone	64091-91-4	2016-09-09

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01
4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone	64091-91-4	2016-09-09

California Prop. 65 Components

	CAS-No.	Revision Date
WARNING! This product contains a chemical known in the State of California to cause cancer.4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanone	64091-91-4	2007-09-28

	CAS-No.	Revision Date
WARNING: This product contains a chemical known in the State of California to cause birth defects or other reproductive harm.Methanol	67-56-1	2012-03-16

SECTION 16: Other information

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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