SAFETY DATA SHEET

Version 6.2
Revision Date 04/23/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : β-Nicotinamide adenine dinucleotide phosphate sodium salt hydrate

Product Number : N0505
Brand : Sigma
CAS-No. : 698999-85-8

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)

Eye irritation (Category 2A), H319

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

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning

Hazard statement(s)
H319 Causes serious eye irritation.

Precautionary statement(s)

P264	Wash skin thoroughly after handling.
P280	Wear eye protection/ face protection.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : Triphosphopyridine nucleotide

Formula : $C_{21}H_{27}N_7NaO_{17}P_3 \cdot xH_2O$

Molecular weight : 765.39 g/mol

Component		Classification	Concentration
Triphosphopyridine nucleotide sodium salt hydrate			
CAS-No.	698999-85-8	Eye Irrit. 2A; H319	<= 100 %
acetone			
CAS-No. EC-No. Index-No. Registration number	67-64-1 200-662-2 606-001-00-8 01-2119471330-49-XXXX	Flam. Liq. 2; Eye Irrit. 2A; STOT SE 3; H225, H319, H336 Concentration limits: >= 20 %: STOT SE 3, H336;	>= 5 - < 10 %

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

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. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
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

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
Nitrogen oxides (NOx)
Oxides of phosphorus
Sodium oxides

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

5.4 Further information
No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

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
Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.**Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Advice on protection against fire and explosion
Provide appropriate exhaust ventilation at places where dust is formed.

Hygiene measures
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Keep container tightly closed in a dry and well-ventilated place.

Storage stability
Recommended storage temperature
-20 °C

Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

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
acetone	67-64-1	TWA	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	500 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		

		TWA	250 ppm 590 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	1,000 ppm 2,400 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	750 ppm 1,800 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	1,000 ppm 2,400 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	750 ppm 1,780 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		C	3,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		PEL	500 ppm 1,200 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Hazardous components without workplace control parameters

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
acetone	67-64-1	Acetone	25 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
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 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: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, 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
Impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator.For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: solid
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: 175 - 178 °C (347 - 352 °F) - lit.
f)	Initial boiling point and boiling range	No data available
g)	Flash point	()No data available
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
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

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
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Strong oxidizing agents

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
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

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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.

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 (Triphosphopyridine nucleotide sodium salt hydrate)

11.2 Additional Information
Not available

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

Dermatitis, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Triphosphopyridine nucleotide sodium salt hydrate)

Stomach - Irregularities - Based on Human Evidence

Kidney - Irregularities - Based on Human Evidence

Skin - Dermatitis - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence
(Triphosphopyridine nucleotide sodium salt hydrate)

Components

Triphosphopyridine nucleotide sodium salt hydrate

Acute toxicity
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

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

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

acetone

Acute toxicity
LD50 Oral - Rat - female - 5,800 mg/kg
Remarks:
(ECHA)
LC50 Inhalation - Rat - 4 h - 76 mg/l
Remarks:
Unconsciousness
Drowsiness
Dizziness
(External MSDS)
LD50 Dermal - Rabbit - 20,000 mg/kg
Remarks:
(IUCLID)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Mild skin irritation - 24 h
(Draize Test)
Remarks:
(RTECS)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Eye irritation - 24 h
(Draize Test)
Remarks:
(RTECS)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: Not a skin sensitizer.
Remarks:
(ECHA)
Chronic exposure may cause dermatitis.

Germ cell mutagenicity

Mutagenicity (mammal cell test): chromosome aberration.
Chinese hamster ovary cells
Result: negative
Ames test
Salmonella typhimurium
Result: negative
In vitro mammalian cell gene mutation test
Mouse lymphoma test
Result: negative

Carcinogenicity

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause drowsiness or dizziness. - Narcotic effects

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 (Triphosphopyridine nucleotide sodium salt hydrate)

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

Triphosphopyridine nucleotide sodium salt hydrate
No data available

acetone

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 6,210 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia pulex (Water flea) - 8,800 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test NOEC - M.aeruginosa - 530 mg/l - 8 d (DIN 38412) Remarks: (maximum permissible toxic concentration) (IUCLID)
Toxicity to bacteria	static test EC50 - activated sludge - 61.15 mg/l - 30 min (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
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)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

Further information
Not classified as dangerous in the meaning of transport regulations.

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
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

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

Massachusetts Right To Know Components

	CAS-No.	Revision Date
acetone	67-64-1	1993-02-16

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Triphosphopyridine nucleotide sodium salt hydrate	698999-85-8	
acetone	67-64-1	1993-02-16

New Jersey Right To Know Components

	CAS-No.	Revision Date
Triphosphopyridine nucleotide sodium salt hydrate	698999-85-8	
acetone	67-64-1	1993-02-16

California Prop. 65 Components
This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

SECTION 16: Other information

Further information

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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