

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Thionicotinamide adenine dinucleotide

Product Number : T7375

Brand : Sigma

CAS-No. : 4090-29-3

#### 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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

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

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



Signal word

Danger

Hazard statement(s)

H370

Causes damage to organs.

Precautionary statement(s)

P260

Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P307 + P311

IF exposed: Call a POISON CENTER or doctor/ physician.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

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

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : Thionicotinamide-DPN

Formula : C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>13</sub>P<sub>2</sub>S

Molecular weight : 679.49 g/mol

CAS-No. : 4090-29-3

#### Hazardous components

| Component            | Classification  | Concentration |
|----------------------|---|---------------|
| <b>Methanol</b>      |   |               |
|                      | Flam. Liq. 2; Acute Tox. 3;<br>STOT SE 1; H225, H301 +<br>H311 + H331, H370 | 1 - 5 %       |
| <b>Acetone</b>       |   |               |
|                      | Flam. Liq. 2; Eye Irrit. 2A;<br>STOT SE 3; H225, H319,<br>H336              | 1 - 5 %       |
| <b>Diethyl ether</b> |   |               |
|                      | Flam. Liq. 1; Acute Tox. 4;<br>STOT SE 3; H224, H302,<br>H336               | 1 - 5 %       |

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

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#### 4. FIRST AID MEASURES

##### 4.1 Description of first aid measures

###### General advice

Consult a physician. Show this 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

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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#### 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

No data available

##### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

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### 6. ACCIDENTAL RELEASE MEASURES

#### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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

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.

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### 7. HANDLING AND STORAGE

#### 7.1 Precautions for safe handling

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

Provide appropriate exhaust ventilation at places where dust is formed.

For precautions see section 2.2.

#### 7.2 Conditions for safe storage, including any incompatibilities

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

Recommended storage temperature -20 °C

Storage class (TRGS 510): 13: Non Combustible Solids

#### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

#### 8.1 Control parameters

##### Components with workplace control parameters

| Component | CAS-No. | Value  | Control parameters | Basis                                   |
|-----------|---------|--|--------------------|---|
| Methanol  | 67-56-1 | TWA  | 200.000000 ppm     | USA. ACGIH Threshold Limit Values (TLV) |
|           | Remarks | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Danger of cutaneous absorption |                    |   |
|           |         | STEL   | 250.000000 ppm     | USA. ACGIH Threshold Limit Values (TLV) |
|           |         | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Danger of cutaneous absorption |                    |   |

|  |  |   |  |   |
|--|--|---|--|---|
|  |  | TWA   | 200.000000<br>ppm<br>260.000000<br>mg/m3 | USA. NIOSH Recommended<br>Exposure Limits   |
|  |  | Potential for dermal absorption   |  |   |
|  |  | ST  | 250.000000<br>ppm<br>325.000000<br>mg/m3 | USA. NIOSH Recommended<br>Exposure Limits   |
|  |  | Potential for dermal absorption   |  |   |
|  |  | TWA   | 200.000000<br>ppm<br>260.000000<br>mg/m3 | USA. Occupational Exposure Limits<br>(OSHA) - Table Z-1 Limits for Air<br>Contaminants        |
|  |  | The value in mg/m3 is approximate.  |  |   |
|  |  | TWA   | 200 ppm                                  | USA. ACGIH Threshold Limit Values<br>(TLV)  |
|  |  | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices<br>(see BEI® section)<br>Danger of cutaneous absorption |  |   |
|  |  | STEL  | 250 ppm                                  | USA. ACGIH Threshold Limit Values<br>(TLV)  |
|  |  | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices<br>(see BEI® section)<br>Danger of cutaneous absorption |  |   |
|  |  | TWA   | 200 ppm<br>260 mg/m3                     | USA. NIOSH Recommended<br>Exposure Limits   |
|  |  | Potential for dermal absorption   |  |   |
|  |  | ST  | 250 ppm<br>325 mg/m3                     | USA. NIOSH Recommended<br>Exposure Limits   |
|  |  | Potential for dermal absorption   |  |   |
|  |  | TWA   | 200 ppm<br>260 mg/m3                     | USA. Occupational Exposure Limits<br>(OSHA) - Table Z-1 Limits for Air<br>Contaminants        |
|  |  | The value in mg/m3 is approximate.  |  |   |
|  |  | STEL  | 250 ppm<br>325 mg/m3                     | USA. OSHA - TABLE Z-1 Limits for<br>Air Contaminants - 1910.1000                              |
|  |  | Skin notation   |  |   |
|  |  | TWA   | 200 ppm<br>260 mg/m3                     | USA. OSHA - TABLE Z-1 Limits for<br>Air Contaminants - 1910.1000                              |
|  |  | Skin notation   |  |   |
|  |  | C   | 1,000 ppm                                | California permissible exposure<br>limits for chemical contaminants<br>(Title 8, Article 107) |
|  |  | Skin  |  |   |
|  |  | PEL   | 200 ppm<br>260 mg/m3                     | California permissible exposure<br>limits for chemical contaminants<br>(Title 8, Article 107) |
|  |  | Skin  |  |   |

|               |         |   |                                      |   |
|---------------|---------|---|--------------------------------------|---|
|               |         | STEL  | 250 ppm<br>325 mg/m3                 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|               |         | Skin  |                                      |   |
| Acetone       | 67-64-1 | TWA   | 250 ppm                              | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>2017 Adoption<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Not classifiable as a human carcinogen |                                      |   |
|               |         | STEL  | 500 ppm                              | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment<br>Upper Respiratory Tract irritation<br>Eye irritation<br>2017 Adoption<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Not classifiable as a human carcinogen |                                      |   |
|               |         | TWA   | 250 ppm<br>590 mg/m3                 | USA. NIOSH Recommended Exposure Limits  |
|               |         | TWA   | 1,000 ppm<br>2,400 mg/m3             | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|               |         | The value in mg/m3 is approximate.  |                                      |   |
|               |         | STEL  | 750 ppm<br>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<br>1,200 mg/m3               | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| Diethyl ether | 60-29-7 | TWA   | 400.000000 ppm                       | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment<br>Upper Respiratory Tract irritation   |                                      |   |
|               |         | STEL  | 500.000000 ppm                       | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment<br>Upper Respiratory Tract irritation   |                                      |   |
|               |         | See Appendix D - Substances with No Established RELs  |                                      |   |
|               |         | TWA   | 400.000000 ppm<br>1,200.000000 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|               |         | The value in mg/m3 is approximate.  |                                      |   |
|               |         | TWA   | 400 ppm                              | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment<br>Upper Respiratory Tract irritation   |                                      |   |
|               |         | STEL  | 500 ppm                              | USA. ACGIH Threshold Limit Values (TLV)   |
|               |         | Central Nervous System impairment   |                                      |   |

|  |  |  |                                    |   |
|--|--|--|------------------------------------|---|
|  |  | Upper Respiratory Tract irritation                   |                                    |   |
|  |  | See Appendix D - Substances with No Established RELs |                                    |   |
|  |  | TWA  | 400 ppm<br>1,200 mg/m <sup>3</sup> | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|  |  | The value in mg/m <sup>3</sup> is approximate.       |                                    |   |
|  |  | TWA  | 400 ppm<br>1,200 mg/m <sup>3</sup> | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                           |
|  |  | STEL   | 500 ppm<br>1,500 mg/m <sup>3</sup> | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                           |
|  |  | PEL  | 400 ppm<br>1,200 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|  |  | STEL   | 500 ppm<br>1,500 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |

#### Biological occupational exposure limits

| Component | CAS-No. | Parameters   | Value        | Biological specimen | Basis                                     |
|-----------|---------|--|--------------|---------------------|---|
|           | -       | Methanol   | 15.0000 mg/l | Urine               | ACGIH - Biological Exposure Indices (BEI) |
|           | Remarks | End of shift (As soon as possible after exposure ceases) |              |                     |   |
|           |         | Methanol   | 15 mg/l      | Urine               | ACGIH - Biological Exposure Indices (BEI) |
|           |         | End of shift (As soon as possible after exposure ceases) |              |                     |   |
|           |         | Acetone  | 25 mg/l      | Urine               | ACGIH - Biological Exposure Indices (BEI) |
|           |         | 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

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.

#### Body Protection

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

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|   |                   |
|---|-------------------|
| a) Appearance                                   | Form: solid       |
| b) Odour  | No data available |
| c) Odour Threshold                              | No data available |
| d) pH   | No data available |
| e) Melting point/freezing point                 | No data available |
| f) Initial boiling point and boiling range      | No data available |
| g) Flash point                                  | Not applicable    |
| h) Evaporation rate                             | No data available |
| i) Flammability (solid, gas)                    | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure                              | No data available |
| l) Vapour 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) Auto-ignition 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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## 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

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides, Oxides of phosphorus

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### 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

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

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.

NTP: No component 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

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

#### Additional Information

RTECS: Not available

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

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

Stomach - Irregularities - Based on Human Evidence

Kidney - Irregularities - Based on Human Evidence

Skin - Dermatitis - Based on Human Evidence

Liver - Ingestion may provoke the following symptoms:; Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Methanol)

Kidney - Irregularities - Based on Human Evidence (Acetone)

Skin - Dermatitis - Based on Human Evidence (Acetone)

Liver - Ingestion may provoke the following symptoms:; Irregularities - Based on Human Evidence (Diethyl ether)

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## 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**

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

**12.6 Other adverse effects**

No data available

**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. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

**14. TRANSPORT INFORMATION**

**DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

**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**

Acute Health Hazard, Chronic Health Hazard

**Reportable Quantity** : F003 lbs

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

|  | CAS-No.   | Revision Date |
|--|-----------|---------------|
| adenosine 5'-(trihydrogen diphosphate), 5'5'-ester with 3-(aminothioxomethyl)-1-β-D-ribofuranosylpyridinium--ate | 4090-29-3 |               |
| Methanol   | 67-56-1   | 2007-07-01    |
| Acetone  | 67-64-1   | 1993-02-16    |
| Diethyl ether  | 60-29-7   | 1993-04-24    |

CAS-No. Revision Date

|  |           |            |
|--|-----------|------------|
| adenosine 5'-(trihydrogen diphosphate), 5'5'-ester with 3-(aminothioxomethyl)-1-β-D-ribofuranosylpyridinium--ate | 4090-29-3 |            |
| Methanol   | 67-56-1   | 2007-07-01 |
| Acetone  | 67-64-1   | 1993-02-16 |
| Diethyl ether  | 60-29-7   | 1993-04-24 |

#### New Jersey Right To Know Components

|  | CAS-No.   | Revision Date |
|--|-----------|---------------|
| adenosine 5'-(trihydrogen diphosphate), 5'5'-ester with 3-(aminothioxomethyl)-1-β-D-ribofuranosylpyridinium--ate | 4090-29-3 |               |
| Methanol   | 67-56-1   | 2007-07-01    |
| Acetone  | 67-64-1   | 1993-02-16    |
| Diethyl ether  | 60-29-7   | 1993-04-24    |

#### California Prop. 65 Components

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

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

|                    |   |
|--------------------|---|
| Acute Tox.         | Acute toxicity  |
| Eye Irrit.         | Eye irritation  |
| Flam. Liq.         | Flammable liquids                                       |
| H224               | Extremely flammable liquid and vapour.                  |
| H225               | Highly flammable liquid and vapour.                     |
| H301 + H311 + H331 | Toxic if swallowed, in contact with skin or if inhaled. |
| H302               | Harmful if swallowed.                                   |
| H319               | Causes serious eye irritation.                          |
| H336               | May cause drowsiness or dizziness.                      |
| H370               | Causes damage to organs (/\$/*_ORGAN_SINGLE\$/).        |
| STOT SE            | Specific target organ toxicity - single exposure        |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: | * |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 0 |
| Reactivity Hazard: | 0 |

### Further information

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**Preparation Information**  
Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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