

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

1.1 Product identifiers

Product name : Isotonitazene HCl
Product Number : I-055

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 Street
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
Specific target organ toxicity - single exposure (Category 1), Eyes, Central nervous system, 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)
H225 : Highly flammable liquid and vapor.
H301 + H311 + H331 : Toxic if swallowed, in contact with skin or if inhaled.

| | |
|----------------------------|--|
| H370 | Causes damage to organs (Eyes, Central nervous system). |
| Precautionary statement(s) | |
| 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. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P310 + P330 | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P307 + P311 | IF exposed: Call a POISON CENTER or doctor/ physician. |
| P362 | Take off contaminated clothing and wash before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| 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. |

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

| Component | | Classification | Concentration |
|---|-----------------------|--|------------------|
| Methanol | | | |
| CAS-No. | 67-56-1 | 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 % |
| EC-No. | 200-659-6 | | |
| Index-No. | 603-001-00-X | | |
| Registration number | 01-2119433307-44-XXXX | | |
| N,N-diethyl-2-[[4-(1-methylethoxy)phenyl]methyl]-5-nitro-1H-Benzimidazole-1-ethanamine hydrochloride (1:1) | | | |
| CAS-No. | 119276-00-5 | Acute Tox. 2; H300 | >= 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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

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

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Mixture with combustible ingredients.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. 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. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature
-25 - 0 °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/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | ST | 250 ppm 325 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | TWA | 200 ppm 260 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | STEL | 250 ppm 325 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | Skin notation | | |
| | | TWA | 200 ppm 260 mg/m ³ | 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/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 250 ppm 325 mg/m ³ | 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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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 | No data available |
| g) Flash point | 9.7 °C (49.5 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| 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

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 99.8 mg/kg
(Calculation method)

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l
(Calculation method)

Acute toxicity estimate Dermal - 300.4 mg/kg
(Calculation method)
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: 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

Mixture causes damage to organs. - Eyes, Central nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Methyl alcohol may be fatal or cause blindness if swallowed.

Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.

Symptoms may be delayed., Damage of the:, Liver, Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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

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

N,N-diethyl-2-[[4-(1-methylethoxy)phenyl]methyl]-5-nitro-1H-Benzimidazole-1-ethanamine hydrochloride (1:1)

Acute toxicity

LD50 Oral - Mouse - 25 mg/kg

Remarks:

(Lit.)

(in analogy to similar products)

The value is given in analogy to the following substances: Diethyl[2-(5-nitro-2-{[4-(propan-2-yloxy)phenyl]methyl}-1H-1,3-benzodiazol-1-yl)ethyl]amine

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

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

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 - <i>Lepomis macrochirus</i> (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA) |
| Toxicity to daphnia and other aquatic invertebrates | semi-static test EC50 - <i>Daphnia magna</i> (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202) |
| Toxicity to algae | static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (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) |

N,N-diethyl-2-[[4-(1-methylethoxy)phenyl]methyl]-5-nitro-1H-Benzimidazole-1-ethanamine hydrochloride (1:1)

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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

This material does not contain any components with a section 302 EHS TPQ.

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 |

Massachusetts Right To Know Components

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

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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Version: 8.0

Revision Date: 04/12/2021

Print Date: 04/15/2021

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

1.1 Product identifiers

Product name : Isotonitazene-13C6 HCl
Product Number : I-057

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 Street
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
Specific target organ toxicity - single exposure (Category 1), Eyes, Central nervous system,
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)
H225 : Highly flammable liquid and vapor.
H301 + H311 + H331 : Toxic if swallowed, in contact with skin or if inhaled.

| | |
|----------------------------|--|
| H370 | Causes damage to organs (Eyes, Central nervous system). |
| Precautionary statement(s) | |
| 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. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P310 + P330 | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P307 + P311 | IF exposed: Call a POISON CENTER or doctor/ physician. |
| P362 | Take off contaminated clothing and wash before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| 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. |

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

| Component | Classification | Concentration |
|---|--|------------------|
| Methanol | | |
| CAS-No. 67-56-1 EC-No. 200-659-6 Index-No. 603-001-00-X Registration number 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 % |
| Diethyl[2-(5-nitro-2-{[4-(propan-2-yloxy)phenyl]methyl})(3a,4,5,6,7,7a-13C6)-1H-1,3-benzodiazol-1-yl]ethyl]amine hydrochloride | | |
| | Acute Tox. 2; H300 | >= 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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

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

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Mixture with combustible ingredients.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. 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. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability

Recommended storage temperature
-25 - 0 °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/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | ST | 250 ppm 325 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | TWA | 200 ppm 260 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | STEL | 250 ppm 325 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | Skin notation | | |
| | | TWA | 200 ppm 260 mg/m ³ | 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/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 250 ppm 325 mg/m ³ | 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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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 | No data available |
| g) Flash point | 9.7 °C (49.5 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| 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

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 99.8 mg/kg
(Calculation method)

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l
(Calculation method)

Acute toxicity estimate Dermal - 300.4 mg/kg
(Calculation method)
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: 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

Mixture causes damage to organs. - Eyes, Central nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Methyl alcohol may be fatal or cause blindness if swallowed.

Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.

Symptoms may be delayed., Damage of the:, Liver, Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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.

I-057

Page 8 of 12

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

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

Diethyl[2-(5-nitro-2-{[4-(propan-2-yloxy)phenyl]methyl})(3a,4,5,6,7,7a-13C6)-1H-1,3-benzodiazol-1-yl]ethyl]amine hydrochloride

Acute toxicity

LD50 Oral - Mouse - 25 mg/kg

Remarks:

(Lit.)

(in analogy to similar products)

The value is given in analogy to the following substances: Diethyl[2-(5-nitro-2-{[4-(propan-2-yloxy)phenyl]methyl}-1H-1,3-benzodiazol-1-yl)ethyl]amine

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

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

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) |

Diethyl[2-(5-nitro-2-{[4-(propan-2-yloxy)phenyl]methyl})(3a,4,5,6,7,7a-13C6)-1H-1,3-benzodiazol-1-yl]ethyl]amine hydrochloride

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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

This material does not contain any components with a section 302 EHS TPQ.

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 |

Massachusetts Right To Know Components

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

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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Version: 8.0

Revision Date: 04/12/2021

Print Date: 04/15/2021

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

1.1 Product identifiers

Product name : N-Phenethyl-4-piperidone (NPP)
Product Number : P-165

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 Street
ST. LOUIS MO 63103
UNITED STATES OF AMERICA (THE)

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 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
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

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapor.
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.

| | |
|----------------------------|--|
| Precautionary statement(s) | |
| 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. |
| P261 | Avoid breathing 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. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P312 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell. |
| 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. |
| P363 | Wash contaminated clothing before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

| Component | Classification | Concentration |
|---------------------|---|------------------|
| Acetonitrile | | |
| CAS-No. | 75-05-8 | >= 90 - <= 100 % |
| EC-No. | 200-835-2 | |
| Index-No. | 608-001-00-3 | |
| Registration number | 01-2119471307-38-XXXX | |
| | | |
| | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302, H332, H312, H319 | |

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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**

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Mixture with combustible ingredients.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. 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. Keep away from heat and sources of ignition.

Storage stability

Recommended storage temperature
-25 - 0 °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 |
|--------------|---------|--|---------------------------------|---|
| Acetonitrile | 75-05-8 | TWA | 20 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Not classifiable as a human carcinogen Danger of cutaneous absorption | | |
| | | TWA | 20 ppm 34 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | TWA | 40 ppm 70 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | TWA | 40 ppm 70 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | STEL | 60 ppm 105 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | PEL | 40 ppm 70 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 60 ppm 105 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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 | No data available |
| g) Flash point | 2.0 °C (35.6 °F) - closed cup |
| 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

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

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

Symptoms: Possible symptoms: , mucosal irritations

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Mixture causes serious 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

11.2 Additional Information

Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components

Acetonitrile

Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l
(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg
(Expert judgment)

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.
(OECD Test Guideline 405)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

Remarks:

(ECHA)

In vitro mammalian cell gene mutation test

Chinese hamster ovary cells

Result: negative

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster ovary cells

Result: Positive results were obtained in some in vitro tests.

Remarks:

(National Toxicology Program)
sister chromatid exchange assay
Chinese hamster ovary cells
Result: negative
Remarks:
Sister chromatid exchange
Saccharomyces cerevisiae
Result: positive
Remarks:
Cytogenetic analysis
(ECHA)
In vitro mammalian cell gene mutation test
Mouse lymphoma test
Result: negative
OECD Test Guideline 474
Mouse - male and female
Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

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

Acetonitrile

| | |
|----------------------|---|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h Remarks: (ECHA) |
| Toxicity to algae | static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253) |
| Toxicity to bacteria | |

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ACETONITRILESOLUTION

IATA

UN number: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

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

| | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01 |

Massachusetts Right To Know Components

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

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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Version: 8.0

Revision Date: 04/28/2021

Print Date: 04/29/2021

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

1.1 Product identifiers

Product name : N-Phenethyl-4-piperidone-13C6 (NPP-13C6)
Product Number : P-167

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 Street
ST. LOUIS MO 63103
UNITED STATES OF AMERICA (THE)

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 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
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

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapor.
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.

| | |
|----------------------------|--|
| Precautionary statement(s) | |
| 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. |
| P261 | Avoid breathing 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. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P312 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell. |
| 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. |
| P363 | Wash contaminated clothing before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

| Component | Classification | Concentration |
|---------------------|---|------------------|
| Acetonitrile | | |
| CAS-No. | 75-05-8 | >= 90 - <= 100 % |
| EC-No. | 200-835-2 | |
| Index-No. | 608-001-00-3 | |
| Registration number | 01-2119471307-38-XXXX | |
| | | |
| | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302, H332, H312, H319 | |

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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**

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Mixture with combustible ingredients.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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. Keep away from heat and sources of ignition.

Storage stability

Recommended storage temperature

-25 - 0 °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 |
|--------------|---------|--|---------------------------------|---|
| Acetonitrile | 75-05-8 | TWA | 20 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Not classifiable as a human carcinogen Danger of cutaneous absorption | | |
| | | TWA | 20 ppm 34 mg/m ³ | USA. NIOSH Recommended Exposure Limits |
| | | TWA | 40 ppm 70 mg/m ³ | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | TWA | 40 ppm 70 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | STEL | 60 ppm 105 mg/m ³ | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | PEL | 40 ppm 70 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 60 ppm 105 mg/m ³ | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

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 | No data available |
| g) Flash point | 2.0 °C (35.6 °F) - closed cup |
| 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

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

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

Symptoms: Possible symptoms: , mucosal irritations

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Mixture causes serious 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

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components

Acetonitrile

Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg
(OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l
(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg
(Expert judgment)

Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.
(OECD Test Guideline 405)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

Remarks:

(ECHA)

In vitro mammalian cell gene mutation test

Chinese hamster ovary cells

Result: negative

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster ovary cells

Result: Positive results were obtained in some in vitro tests.

Remarks:

(National Toxicology Program)
sister chromatid exchange assay
Chinese hamster ovary cells
Result: negative
Remarks:
Sister chromatid exchange
Saccharomyces cerevisiae
Result: positive
Remarks:
Cytogenetic analysis
(ECHA)
In vitro mammalian cell gene mutation test
Mouse lymphoma test
Result: negative
OECD Test Guideline 474
Mouse - male and female
Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

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

Acetonitrile

| | |
|----------------------|---|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h Remarks: (ECHA) |
| Toxicity to algae | static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253) |
| Toxicity to bacteria | |

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ACETONITRILESOLUTION

IATA

UN number: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

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

| | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01 |

Massachusetts Right To Know Components

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

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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