



3-BUTENENITRILE

Safety Data Sheet ENEB0575

Date of issue: 01/26/2015

Revision date: 08/31/2015

Version: 2.0

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

1.1. Product identifier

Product form : Substance
 Physical state : Liquid
 Substance name : 3-BUTENENITRILE
 Product code : ENEB0575
 Formula : C4H5N
 Synonyms : ALLYL CYANIDE; VINYLACETONITRILE
 Chemical family : ORGANONITRILE

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

Use of the substance/mixture : Chemical intermediate
 For research and industrial use only

1.3. Details of the supplier of the safety data sheet

GELEST, INC.

11 East Steel Road
 Morrisville, PA 19067

USA

T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST

info@gelest.com - www.gelest.com

1.4. Emergency telephone number

Emergency number : CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Flam. Liq. 3 H226
 Acute Tox. 3 (Oral) H301
 Acute Tox. 4 (Dermal) H312
 Skin Irrit. 2 H315
 Eye Irrit. 2A H319
 STOT SE 3 H335

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H226 - Flammable liquid and vapor
 H301 - Toxic if swallowed
 H312 - Harmful in contact with skin
 H315 - Causes skin irritation
 H319 - Causes serious eye irritation
 H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P280 - Wear protective gloves/protective clothing/eye protection/face protection
 P210 - Keep away from heat, open flames, sparks. - No smoking
 P240 - Ground/bond container and receiving equipment
 P241 - Use explosion-proof electrical equipment
 P242 - Use only non-sparking tools
 P243 - Take precautionary measures against static discharge
 P261 - Avoid breathing vapors
 P264 - Wash hands thoroughly after handling
 P270 - Do not eat, drink or smoke when using this product
 P271 - Use only outdoors or in a well-ventilated area
 P330 - Rinse mouth
 P301+P310 - If swallowed: Immediately call a doctor

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P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing. rinse skin with water/shower
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P312 - Call a doctor if you feel unwell
P332+P313 - If skin irritation occurs: Get medical advice/attention
P337+P313 - If eye irritation persists: Get medical advice/attention
P362 - Take off contaminated clothing and wash before reuse
P370+P378 - In case of fire: Use water spray, foam, carbon dioxide, dry chemical to extinguish
P403+P233 - Store in a well-ventilated place. Keep container tightly closed
P403+P235 - Keep in a cool place
P405 - Store locked up
P501 - Dispose of contents/container to licensed waste disposal facility.

2.3. Other hazards

No additional information available

2.4. Unknown acute toxicity (GHS US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Substance type : Multi-constituent
Name : 3-BUTENENITRILE
CAS No : 109-75-1
EC no : 203-701-1

| Name | Product identifier | % | Classification (GHS-US) |
|-----------------|--------------------|----------|---|
| 3-Butenenitrile | (CAS No) 109-75-1 | 95 - 100 | Flam. Liq. 3, H226 Acute Tox. 3 (Oral), H301 Acute Tox. 4 (Dermal), H312 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335 |
| 2-Butenenitrile | (CAS No) 4786-20-3 | 0 - 1 | Flam. Liq. 2, H225 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335 |

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact : Wash with plenty of soap and water. Get medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Get medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/injuries after inhalation : May cause respiratory irritation. Overexposure may cause: Coughing. Headache. Nausea.

Symptoms/injuries after skin contact : Causes skin irritation. Harmful in contact with skin.

Symptoms/injuries after eye contact : Causes serious eye irritation.

Symptoms/injuries after ingestion : Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard.

Chronic symptoms : Nitriles may be partially metabolized to cyanide in the body. Symptoms of cyanide exposure include rapid respiration, gasping, headache, drop in blood pressure, vomiting, loss of consciousness and death.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Water spray. Foam. Carbon dioxide. Dry chemical.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Flammable liquid and vapor. Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

5.3. Advice for firefighters

Firefighting instructions : Use water spray to cool exposed surfaces. Exercise caution when fighting any chemical fire.
Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Avoid all eye and skin contact and do not breathe vapor and mist.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. Use special care to avoid static electric charges.

6.1.1. For non-emergency personnel

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Clean up any spills as soon as possible, using an absorbent material to collect it. Sweep or shovel spills into appropriate container for disposal. Use only non-sparking tools.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Use only outdoors or in a well-ventilated area. Avoid breathing vapors. Provide good ventilation in process area to prevent accumulation of vapors. Containers must be properly grounded before beginning transfer. Take precautionary measures against static discharge. Use only non-sparking tools.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep container tightly closed.
Incompatible materials : Acids. Alcohols. Oxidizing agent. Peroxides.
Storage area : Store in a well-ventilated place. Store away from heat.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

3-Butenenitrile (109-75-1)

| | | |
|-----------|-----------------|------------------------------------|
| USA ACGIH | ACGIH TWA (ppm) | 10 ppm Gelest recommended TLV 8 Hr |
|-----------|-----------------|------------------------------------|

8.2. Exposure controls

Appropriate engineering controls : Provide local exhaust or general room ventilation.
Personal protective equipment : Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

Hand protection : Neoprene or nitrile rubber gloves.

Eye protection : Chemical goggles. Contact lenses should not be worn.

Skin and body protection : Wear suitable protective clothing.

Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified combination organic vapor - amine gas (brown cartridge) respirator.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|---|-------------------------------|
| Physical state | : Liquid |
| Appearance | : Clear liquid. |
| Molecular mass | : 67.09 g/mol |
| Color | : Amber. |
| Odor | : Distinct. |
| Odor threshold | : No data available |
| Refractive index | : 1.405 |
| pH | : No data available |
| Relative evaporation rate (butyl acetate=1) | : ~ 1 |
| Melting point | : No data available |
| Freezing point | : < -87 °C |
| Boiling point | : 116 - 119 °C |
| Flash point | : 24 °C |
| Auto-ignition temperature | : No data available |
| Decomposition temperature | : No data available |
| Flammability (solid, gas) | : Flammable liquid and vapor |
| Vapor pressure | : ~ 30 mm Hg @ 13°C |
| Relative vapor density at 20 °C | : 2.3 |
| Relative density | : 0.834 |
| VOC content | : 100 % |
| Solubility | : Slightly. Soluble in water. |
| Log Pow | : No data available |
| Log Kow | : No data available |
| Viscosity, kinematic | : No data available |
| Viscosity, dynamic | : No data available |
| Explosive properties | : No data available |
| Oxidizing properties | : No data available |
| Explosion limits | : No data available |

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable when stored in sealed containers.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Air. Heat. Open flame. Sparks. Direct sunlight.

10.5. Incompatible materials

Acids. Alcohols. Peroxides. Oxidizing agent.

10.6. Hazardous decomposition products

Organic amine vapors.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Toxic if swallowed. Dermal: Harmful in contact with skin.

| 3-BUTENENITRILE (109-75-1) | |
|-----------------------------------|---------------------------|
| LD50 oral rat | 115 mg/kg |
| 3-Butenenitrile (109-75-1) | |
| LD50 oral rat | 115 mg/kg |
| LD50 dermal rabbit | 1176 mg/kg |
| ATE US (oral) | 115.000 mg/kg body weight |

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| 3-Butenenitrile (109-75-1) | |
|--|---|
| ATE US (dermal) | 1176.000 mg/kg body weight |
| 2-Butenenitrile (4786-20-3) | |
| LD50 oral rat | 501 mg/kg |
| LD50 oral mouse | 396 mg/kg |
| LD50 oral guinea pig | 272 |
| ATE US (oral) | 501.000 mg/kg body weight |
| Skin corrosion/irritation | : Causes skin irritation. |
| Serious eye damage/irritation | : Causes serious eye irritation. |
| Respiratory or skin sensitization | : Not classified |
| Germ cell mutagenicity | : Not classified |
| Carcinogenicity | : Not classified |
| Reproductive toxicity | : Not classified |
| Specific target organ toxicity (single exposure) | : May cause respiratory irritation. |
| Specific target organ toxicity (repeated exposure) | : Not classified |
| Aspiration hazard | : Not classified |
| Symptoms/injuries after inhalation | : May cause respiratory irritation. Overexposure may cause: Coughing. Headache. Nausea. |
| Symptoms/injuries after skin contact | : Causes skin irritation. Harmful in contact with skin. |
| Symptoms/injuries after eye contact | : Causes serious eye irritation. |
| Symptoms/injuries after ingestion | : Toxic if swallowed. Swallowing a small quantity of this material will result in serious health hazard. |
| Chronic symptoms | : Nitriles may be partially metabolized to cyanide in the body. Symptoms of cyanide exposure include rapid respiration, gasping, headache, drop in blood pressure, vomiting, loss of consciousness and death. |
| Reason for classification | : Expert judgment |

SECTION 12: Ecological information

12.1. Toxicity

| 3-Butenenitrile (109-75-1) | |
|-----------------------------------|--|
| LC50 fish 1 | 171 - 195 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through]) |

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

| | |
|------------------------------|---|
| Other adverse effects | : This substance may be hazardous to the environment. |
| Effect on ozone layer | : No additional information available |
| Effect on the global warming | : No known ecological damage caused by this product. |

SECTION 13: Disposal considerations

13.1. Waste treatment methods

| | |
|--------------------------------|--|
| Waste disposal recommendations | : May be incinerated. Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility. |
| Ecology - waste materials | : Avoid release to the environment. |

SECTION 14: Transport information

14.1. UN number

| | |
|-------------|--------|
| UN-No.(DOT) | : 2929 |
| DOT NA no. | UN2929 |

14.2. UN proper shipping name

| | |
|---|--|
| Proper Shipping Name (DOT) | : Toxic liquids, flammable, organic, n.o.s. (3-BUTENENITRILE) |
| Department of Transportation (DOT) Hazard Classes | : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132 |

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Hazard labels (DOT) : 6.1 - Poison
3 - Flammable liquid



DOT Symbols : G - Identifies PSN requiring a technical name
Packing group (DOT) : II - Medium Danger
DOT Packaging Exceptions (49 CFR 173.xxx) : 153
DOT Packaging Non Bulk (49 CFR 173.xxx) : 202
DOT Packaging Bulk (49 CFR 173.xxx) : 243

14.3. Additional information

Other information : No supplementary information available.

Transport by sea

DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

DOT Vessel Stowage Other : 40 - Stow "clear of living quarters"

Air transport

DOT Quantity Limitations Passenger aircraft/rail : 5 L
(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 60 L
CFR 175.75)

SECTION 15: Regulatory information

15.1. US Federal regulations

3-Butenenitrile (109-75-1)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

2-Butenenitrile (4786-20-3)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations

3-Butenenitrile (109-75-1)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on the Canadian NDSL (Non-Domestic Substances List)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Japanese Poisonous and Deleterious Substances Control Law

2-Butenenitrile (4786-20-3)

Listed on the Canadian NDSL (Non-Domestic Substances List)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on the Japanese ISHL (Industrial Safety and Health Law)
Listed on the Korean ECL (Existing Chemicals List)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Japanese Poisonous and Deleterious Substances Control Law
Listed on INSQ (Mexican national Inventory of Chemical Substances)

15.3. US State regulations

3-BUTENENITRILE(109-75-1)

| | |
|---|----|
| U.S. - California - Proposition 65 - Carcinogens List | No |
| U.S. - California - Proposition 65 - Developmental Toxicity | No |
| U.S. - California - Proposition 65 - Reproductive Toxicity - Female | No |
| U.S. - California - Proposition 65 - Reproductive Toxicity - Male | No |

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| 3-Butenenitrile (109-75-1) | | | | |
|---|---|---|---|-----------------------------------|
| U.S. - California - Proposition 65 - Carcinogens List | U.S. - California - Proposition 65 - Developmental Toxicity | U.S. - California - Proposition 65 - Reproductive Toxicity - Female | U.S. - California - Proposition 65 - Reproductive Toxicity - Male | No significance risk level (NSRL) |
| No | No | No | No | |
| 2-Butenenitrile (4786-20-3) | | | | |
| U.S. - California - Proposition 65 - Carcinogens List | U.S. - California - Proposition 65 - Developmental Toxicity | U.S. - California - Proposition 65 - Reproductive Toxicity - Female | U.S. - California - Proposition 65 - Reproductive Toxicity - Male | No significance risk level (NSRL) |
| No | No | No | No | |

SECTION 16: Other information

Abbreviations and acronyms

: Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development.

Full text of H-phrases::

| | |
|-----------------------|---|
| Acute Tox. 3 (Oral) | Acute toxicity (oral) Category 3 |
| Acute Tox. 4 (Dermal) | Acute toxicity (dermal) Category 4 |
| Acute Tox. 4 (Oral) | Acute toxicity (oral) Category 4 |
| Eye Irrit. 2A | Serious eye damage/eye irritation Category 2A |
| Flam. Liq. 2 | Flammable liquids Category 2 |
| Flam. Liq. 3 | Flammable liquids Category 3 |
| Skin Irrit. 2 | Skin corrosion/irritation Category 2 |
| STOT SE 3 | Specific target organ toxicity (single exposure) Category 3 |
| H225 | Highly flammable liquid and vapor |
| H226 | Flammable liquid and vapor |
| H301 | Toxic if swallowed |
| H302 | Harmful if swallowed |
| H312 | Harmful in contact with skin |
| H315 | Causes skin irritation |
| H319 | Causes serious eye irritation |
| H335 | May cause respiratory irritation |

HMIS III Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
Flammability : 3 Serious Hazard
Physical : 0 Minimal Hazard

Prepared by safety and environmental affairs.

Date of issue: 01/26/2015 Revision date: 08/31/2015 Version: 2.0

SDS US (GHS HazCom 2012) - Custom

According to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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