SECTION 1: Identification

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

1.2. Recommended use and restrictions on use
Recommended use: Chemical intermediate

1.3. Supplier
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: Hazard(s) identification

2.1. Classification of the substance or mixture
GHS-US classification
Flammable liquids Category 3
Acute toxicity (oral) Category 3
Acute toxicity (dermal) Category 4
Skin corrosion/irritation Category 2
Serious eye damage/eye irritation Category 2A
Specific target organ toxicity (single exposure) Category 3

Full text of H statements: see section 16

2.2. GHS Label elements, including precautionary statements
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
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.
**3-BUTENENITRILE**

**Safety Data Sheet**

---

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.

P403+P233 - Store in a well-ventilated place. Keep container tightly closed.

P403+P235 - Keep in a cool place

P501 - Dispose of contents/container to licensed waste disposal facility.

---

2.3. **Hazards not otherwise classified (HNOC)**

No additional information available

2.4. **Unknown acute toxicity (GHS US)**

Not applicable

**SECTION 3: Composition/Information on ingredients**

3.1. **Substances**

<table>
<thead>
<tr>
<th>Name</th>
<th>Product identifier</th>
<th>%</th>
<th>GHS-US classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-Butenenitrile</td>
<td>(CAS-No.) 109-75-1</td>
<td>95 - 100</td>
<td>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</td>
</tr>
<tr>
<td>2-Butenenitrile</td>
<td>(CAS-No.) 4786-20-3</td>
<td>0 - 1</td>
<td>Flam. Liq. 2, H225 \ Acute Tox. 4 (Oral), H302 \ Skin Irrit. 2, H315 \ Eye Irrit. 2A, H319 \ STOT SE 3, H335</td>
</tr>
</tbody>
</table>

---

**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 (acute and delayed)**


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

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

Symptoms/effects 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. **Immediate medical attention and special treatment, if necessary**

No additional information available

**SECTION 5: Fire-fighting measures**

5.1. **Suitable (and unsuitable) extinguishing media**


5.2. **Specific hazards arising from the chemical**

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. Special protective equipment and precautions for fire-fighters

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.


Storage area: Store in a well-ventilated place. Store away from heat.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

<table>
<thead>
<tr>
<th>3-Butenenitrile (109-75-1)</th>
<th>ACGIH</th>
<th>ACGIH TWA (ppm)</th>
<th>10 ppm Gelest recommended TLV 8 Hr</th>
</tr>
</thead>
</table>

8.2. Appropriate engineering controls

Appropriate engineering controls: Provide local exhaust or general room ventilation.

8.3. Individual protection measures/Personal protective equipment

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.
SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

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

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


10.5. Incompatible materials


10.6. Hazardous decomposition products

Organic amine vapors.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

**3-BUTENENITRILE (109-75-1)**

<table>
<thead>
<tr>
<th>Route</th>
<th>LD50 Oral rat</th>
<th>LD50 Dermal rabbit</th>
<th>ATE US (oral)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral rat</td>
<td>115 mg/kg</td>
<td>1176 mg/kg</td>
<td>115 mg/kg body weight</td>
</tr>
</tbody>
</table>

**3-Butenenitrile (109-75-1)**
### 3-Butenenitrile (109-75-1)

**ATE US (dermal)**
1176 mg/kg body weight

### 2-Benzylpropanenitrile (4786-20-3)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>LD50 oral rat</td>
<td>501 mg/kg</td>
</tr>
<tr>
<td>LD50 oral mouse</td>
<td>396 mg/kg</td>
</tr>
<tr>
<td>LD50 oral guinea pig</td>
<td>272</td>
</tr>
<tr>
<td>ATE US (oral)</td>
<td>501 mg/kg body weight</td>
</tr>
</tbody>
</table>

**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/effects after inhalation**

**Symptoms/effects after skin contact**
Causes skin irritation. Harmful in contact with skin.

**Symptoms/effects after eye contact**
Causes serious eye irritation.

**Symptoms/effects 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)**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>LC50 fish</td>
<td>171 - 195 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])</td>
</tr>
</tbody>
</table>

#### 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 the ozone layer
No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Disposal methods

**Product/Packaging 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

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>UN-No.(DOT)</td>
<td>2929</td>
</tr>
<tr>
<td>DOT NA no.</td>
<td>UN2929</td>
</tr>
</tbody>
</table>

#### 14.2. UN proper shipping name

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Transport document description</td>
<td>UN2929 Toxic liquids, flammable, organic, n.o.s. (3-BUTENENITRILE), 6.1 (3), II</td>
</tr>
<tr>
<td>Proper Shipping Name (DOT)</td>
<td>Toxic liquids, flammable, organic, n.o.s. (3-BUTENENITRILE)</td>
</tr>
</tbody>
</table>
3-BUTENENITRILE
Safety Data Sheet

Packing group (DOT) : II - Medium Danger
Hazard labels (DOT) : 6.1 - Poison
3 - Flammable liquid

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

14.3. Additional information
Emergency Response Guide (ERG) Number : 131
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 (49 CFR 173.27) : 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 60 L

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

CANADA

3-Butenenitrile (109-75-1)
Listed on the Canadian NDSL (Non-Domestic Substances List)

2-Butenenitrile (4786-20-3)
Listed on the Canadian NDSL (Non-Domestic Substances List)

EU-Regulations

3-Butenenitrile (109-75-1)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

2-Butenenitrile (4786-20-3)
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

National regulations

3-Butenenitrile (109-75-1)
Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on NZIoC (New Zealand Inventory of Chemicals)
Japanese Poisonous and Deleterious Substances Control Law
3-BUTENENITRILE
Safety Data Sheet

2-Butenenitrile (4786-20-3)
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
California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

2-Butenenitrile (4786-20-3)
U.S. - New Jersey - Right to Know Hazardous Substance List

SECTION 16: Other information
Full text of H-phrases:

| 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 |

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; GHS: The Globally Harmonized System of Classification and Labelling; APF: Assigned Protection Factor.

Hazard Rating
Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
Flammability : 3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F. as well as liquids with flash points between 73 F and 100 F. (Classes IB & IC)
Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

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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