



## 2-METHYL-3-BUTENENITRILE, tech-95

Safety Data Sheet ENEM2120

Date of issue: 12/28/2016 Version: 1.0

### SECTION 1: Identification

#### 1.1. Product identifier

Product name : 2-METHYL-3-BUTENENITRILE, tech-95  
 Product code : ENEM2120  
 Product form : Substance  
 Physical state : Liquid  
 Formula : C5H7N  
 Synonyms : ALLYL CYANIDE; VINYLACETONITRILE  
 Chemical family : ORGANONITRILE

#### 1.2. Recommended use of the chemical and restrictions on use

Recommended use : 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](mailto:info@gelest.com) - [www.gelest.com](http://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 2 H225  
 Acute toxicity (oral) Category 3 H301  
 Acute toxicity (dermal) Category 3 H311  
 Acute toxicity (inhalation:vapor) Category 3 H331  
 Full text of H statements : see section 16

#### 2.2. Label elements

##### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS02

GHS06

Signal word (GHS-US) : Danger  
 Hazard statements (GHS-US) : H225 - Highly flammable liquid and vapor  
 H301+H311+H331 - Toxic if swallowed, in contact with skin or if inhaled  
 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  
 P312 - Call a doctor if you feel unwell  
 P321 - Specific treatment (see first aid instructions on this label)  
 P361 - Take off immediately all contaminated clothing

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P363 - Wash contaminated clothing 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. Hazards not otherwise classified (HNOC)

Other hazards not contributing to the classification : Gelested recommended TLV 10ppm 8 Hr. TWA.

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

No data available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Substance type : Multi-constituent  
Name : 2-METHYL-3-BUTENENITRILE, tech-95  
CAS No : 16529-56-9

Name	Product identifier	%	GHS-US classification
2-Methyl-3-butenenitrile	(CAS No) 16529-56-9	75 - 100	Flam. Liq. 2, H225 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Inhalation:vapour), H331
3-Pentenitrile	(CAS No) 4635-87-4	0 - 15	Flam. Liq. 3, H226 Acute Tox. 4 (Oral), H302 Acute Tox. 2 (Inhalation), H330
2-Methyl-2-buteniyrile	(CAS No) 4403-61-6	0 - 10	Flam. Liq. 2, H225 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Inhalation), H331
4-Pentenitrile	(CAS No) 592-51-8	0 - 5	Flam. Liq. 3, H226 Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Acute Tox. 4 (Inhalation), H332

Full text of hazard classes and H-statements : see section 16

### 3.2. Mixtures

Not applicable

### 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. Immediately call a poison center or doctor/physician.

First-aid measures after skin contact : Wash with plenty of soap and water. Immediately call a poison center or doctor/physician.

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. Immediately call a poison center or doctor/physician.

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

Symptoms/injuries after inhalation : May cause irritation to the respiratory tract.

Symptoms/injuries after skin contact : Toxic in contact with skin. May cause skin irritation. Skin permeation may occur in amounts producing the effects of systemic toxicity.

Symptoms/injuries after eye contact : May cause 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

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

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

Unsuitable extinguishing media : None known.

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### 5.2. Special hazards arising from the substance or mixture

- Fire hazard : Highly flammable liquid and vapor. Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.
- Explosion hazard : May form flammable/explosive vapor-air mixture.

### 5.3. Advice for firefighters

- Firefighting instructions : Exercise caution when fighting any chemical fire. Use water spray to cool exposed surfaces.
- 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 : Eliminate every possible source of ignition. Use special care to avoid static electric charges.

#### 6.1.1. For non-emergency personnel

- Protective equipment : Wear protective equipment as described in Section 8.
- Emergency procedures : Evacuate unnecessary personnel.

#### 6.1.2. For emergency responders

- Protective equipment : Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: "Exposure controls/personal 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

- For containment : Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.
- Methods for cleaning up : Clean up any spills as soon as possible, using an absorbent material to collect it. 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

- Additional hazards when processed : Handle empty containers with care because residual vapors are flammable. Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
- Precautions for safe handling : Avoid all eye and skin contact and do not breathe vapor and mist. Ground/bond container and receiving equipment. Take precautionary measures against static discharge. Use only outdoors or in a well-ventilated area. Use only non-sparking tools.
- Hygiene measures : Wash contaminated clothing before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

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

- Technical measures : Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.
- Storage conditions : Keep container tightly closed. Keep in a cool place.
- Incompatible materials : Acids. Alcohols. Oxidizing agent. Peroxides.
- Storage area : Store in a well-ventilated place. Store away from heat.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

- No additional information available

### 8.2. Exposure controls

- Appropriate engineering controls : Handle in an enclosing hood with exhaust 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.

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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

Physical state	: Liquid
Appearance	: Clear liquid.
Molecular mass	: 81.11 g/mol
Color	: Amber.
Odor	: Distinct.
Odor threshold	: No data available
Refractive index	: No data available
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: ~ 1
Melting point	: No data available
Freezing point	: < 0 °C
Boiling point	: 124 °C
Flash point	: 15 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Highly flammable liquid and vapor
Vapor pressure	: 13.1 mm Hg @ 13°C
Relative vapor density at 20 °C	: > 1
Relative density	: 0.82
VOC content	: < 40 %
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

Heat. Open flame. Sparks.

#### 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: Toxic in contact with skin. Inhalation:vapour: Toxic if inhaled.

#### 2-METHYL-3-BUTENENITRILE, tech-95 (16529-56-9)

ATE US (oral)	175.121 mg/kg body weight
ATE US (dermal)	407.585 mg/kg body weight

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ATE US (vapors)	3.000 mg/l/4h
<b>2-Methyl-3-butenenitrile (16529-56-9)</b>	
LD50 oral rat	232 mg/kg
LD50 dermal rabbit	482 mg/kg
LC50 inhalation rat (ppm)	3000 ppm/4h
ATE US (oral)	232.000 mg/kg body weight
ATE US (dermal)	482.000 mg/kg body weight
ATE US (gases)	3000.000 ppmV/4h
ATE US (vapors)	3.000 mg/l/4h
<b>3-Pentenitrile (4635-87-4)</b>	
LC50 inhalation rat	420 ppm/4h
LDLo inhalation rat	300 mg/kg
ATE US (oral)	500.000 mg/kg body weight
ATE US (gases)	100.000 ppmV/4h
ATE US (vapors)	0.500 mg/l/4h
ATE US (dust, mist)	0.050 mg/l/4h
<b>2-Methyl-2-butenitrile (4403-61-6)</b>	
LC50 inhalation rat	420 ppm/4h
ATE US (oral)	100.000 mg/kg body weight
ATE US (dermal)	300.000 mg/kg body weight
ATE US (gases)	700.000 ppmV/4h
ATE US (vapors)	3.000 mg/l/4h
ATE US (dust, mist)	0.500 mg/l/4h
<b>4-Pentenitrile (592-51-8)</b>	
LC50 inhalation rat	2550 ppm/4h
LDLo inhalation rat	2250 mg/kg
ATE US (oral)	500.000 mg/kg body weight
ATE US (dermal)	1100.000 mg/kg body weight
ATE US (gases)	4500.000 ppmV/4h
ATE US (vapors)	11.000 mg/l/4h
ATE US (dust, mist)	1.500 mg/l/4h
Skin corrosion/irritation	: Not classified
Serious eye damage/irritation	: Not classified
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
	None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen
Reproductive toxicity	: Not classified
Specific target organ toxicity – single exposure	: Not classified
Specific target organ toxicity – repeated exposure	: Not classified
Aspiration hazard	: Not classified
Symptoms/injuries after inhalation	: May cause irritation to the respiratory tract.
Symptoms/injuries after skin contact	: Toxic in contact with skin. May cause skin irritation. Skin permeation may occur in amounts producing the effects of systemic toxicity.
Symptoms/injuries after eye contact	: May cause 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

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### SECTION 12: Ecological information

#### 12.1. Toxicity

No additional information available

#### 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 effects from this product.  
GWPmix comment : No known effects from this product.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Sewage disposal recommendations : Do not dispose of waste into sewer.  
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.  
Additional information : Handle empty containers with care because residual vapors are flammable.  
Ecology - waste materials : Avoid release to the environment.

### SECTION 14: Transport information

#### 14.1. UN number

UN-No.(DOT) : 1992  
DOT NA no. UN1992

#### 14.2. UN proper shipping name

Transport document description : UN1992 Flammable liquids, toxic, n.o.s. (2-METHYL-3-BUTENENITRILE), 3 (6.1), II  
Proper Shipping Name (DOT) : Flammable liquids, toxic, n.o.s.  
(2-METHYL-3-BUTENENITRILE)  
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120  
Packing group (DOT) : II - Medium Danger  
Hazard labels (DOT) : 3 - Flammable liquid  
6.1 - Poison



DOT Packaging Non Bulk (49 CFR 173.xxx) : 202  
DOT Packaging Bulk (49 CFR 173.xxx) : 243  
DOT Packaging Exceptions (49 CFR 173.xxx) : 150  
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"

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### Air transport

DOT Quantity Limitations Passenger aircraft/rail : 1 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

#### 2-Methyl-3-butenenitrile (16529-56-9)

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

#### 3-Pentenitrile (4635-87-4)

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

#### 2-Methyl-2-buteniyirile (4403-61-6)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

#### 4-Pentenitrile (592-51-8)

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

### 15.2. International regulations

#### CANADA

#### 2-Methyl-3-butenenitrile (16529-56-9)

Listed on the Canadian NDSL (Non-Domestic Substances List)

#### 3-Pentenitrile (4635-87-4)

Listed on the Canadian NDSL (Non-Domestic Substances List)

#### 4-Pentenitrile (592-51-8)

Listed on the Canadian NDSL (Non-Domestic Substances List)

#### EU-Regulations

#### 2-Methyl-3-butenenitrile (16529-56-9)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### 3-Pentenitrile (4635-87-4)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### 2-Methyl-2-buteniyirile (4403-61-6)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### 4-Pentenitrile (592-51-8)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### National regulations

#### 2-Methyl-3-butenenitrile (16529-56-9)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Japanese Poisonous and Deleterious Substances Control Law

#### 3-Pentenitrile (4635-87-4)

Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory  
Listed on the Korean ECL (Existing Chemicals List)

#### 2-Methyl-2-buteniyirile (4403-61-6)

Listed on the AICS (Australian Inventory of Chemical Substances)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

### 15.3. US State regulations

No additional information available

## 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

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H311	Toxic in contact with skin
H312	Harmful in contact with skin
H330	Fatal if inhaled
H331	Toxic if inhaled
H332	Harmful if inhaled

### 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.

### HMIS III 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: 12/28/2016 Version: 1.0

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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