

### SECTION 1: Identification

#### 1.1. Identification

Product form : Substance  
 Substance name : Hexafluoroacetone sesquideuterate  
 CAS-No. : 62251-10-9  
 Product code : 2117-3-90  
 Other means of identification : MFCD00149064

#### 1.2. Recommended use and restrictions on use

Use of the substance/mixture : Laboratory chemicals  
 Manufacture of substances  
 Scientific research and development

#### 1.3. Supplier

SynQuest Laboratories, Inc. Inc.  
 P.O. Box 309  
 Alachua, FL, Alachua, 32615  
 United States of America  
 T (386) 462-0788 - F (386) 462-7097  
[info@synquestlabs.com](mailto:info@synquestlabs.com) - [www.synquestlabs.com](http://www.synquestlabs.com)

#### 1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### GHS US classification

|   |      |  |
|---|------|--|
| Acute toxicity (oral) Category 3  | H301 | Toxic if swallowed                       |
| Acute toxicity (dermal) Category 3  | H311 | Toxic in contact with skin               |
| Skin corrosion/irritation Category 1B   | H314 | Causes severe skin burns and eye damage  |
| Serious eye damage/eye irritation Category 2A   | H319 | Causes serious eye irritation            |
| Reproductive toxicity Category 1B   | H360 | May damage fertility or the unborn child |
| Specific target organ toxicity – Single exposure, Category 3,<br>Respiratory tract irritation | H335 | May cause respiratory irritation         |

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) :

H301+H311 - Toxic if swallowed or in contact with skin  
 H314 - Causes severe skin burns and eye damage  
 H319 - Causes serious eye irritation

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### Precautionary statements (GHS US)

H335 - May cause respiratory irritation  
H360 - May damage fertility or the unborn child  
: P201 - Obtain special instructions before use.  
P202 - Do not handle until all safety precautions have been read and understood.  
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/protective clothing/eye protection/face protection.  
P301+P310 - If swallowed: Immediately call a poison center or doctor.  
P301+P330+P331 - If swallowed: rinse mouth. Do NOT induce vomiting.  
P302+P352 - If on skin: Wash with plenty of soap and water  
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.  
P308+P313 - If exposed or concerned: Get medical advice/attention.  
P310 - Immediately call a POISON CENTER or doctor/ physician  
P321 - Specific treatment (see supplemental first aid instructions on this label)  
P322 - Specific treatment (see supplemental first aid instruction on this label)  
P330 - Rinse mouth.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P361+P364 - Take off immediately all contaminated clothing and wash it before reuse.  
P363 - Wash contaminated clothing before reuse.  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.  
P405 - Store locked up.  
P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards which do not result in classification

No additional information available

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

Not applicable

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Name : Hexafluoroacetone sesquideuterate  
CAS-No. : 62251-10-9

| Name              | Product identifier | %  | GHS US classification  |
|-------------------|--------------------|----|--|
| Hexafluoroacetone | CAS-No.: 684-16-2  | 86 | Press. Gas (Liq.), H280<br>Acute Tox. 3 (Oral), H301<br>Acute Tox. 3 (Dermal), H311<br>Acute Tox. 2 (Inhalation), H330<br>Skin Corr. 1B, H314<br>Eye Dam. 1, H318<br>Repr. 1B, H360<br>STOT SE 3, H335 |
| Deuterium oxide   | CAS-No.: 7789-20-0 | 14 | Not classified   |

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

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### 3.2. Mixtures

Not applicable

## SECTION 4: First-aid measures

### 4.1. Description of first aid measures

|                                       |   |
|---------------------------------------|---|
| First-aid measures general            | : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.          |
| First-aid measures after inhalation   | : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.                             |
| First-aid measures after skin contact | : Wash with plenty of soap and water. Get immediate 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 immediate medical advice/attention. |
| First-aid measures after ingestion    | : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.                                |

### 4.2. Most important symptoms and effects (acute and delayed)

|                  |  |
|------------------|--|
| Symptoms/effects | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11. |
|------------------|--|

### 4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

## SECTION 5: Fire-fighting measures

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

|                              |  |
|------------------------------|--|
| Suitable extinguishing media | : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire. |
|------------------------------|--|

### 5.2. Specific hazards arising from the chemical

|             |  |
|-------------|--|
| Fire hazard | : Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. |
|-------------|--|

### 5.3. Special protective equipment and precautions for fire-fighters

|                                |  |
|--------------------------------|--|
| Firefighting instructions      | : In case of fire: Evacuate area.  |
| Protection during firefighting | : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection". |

## SECTION 6: Accidental release measures

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

|                  |   |
|------------------|---|
| General measures | : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe gas, fumes, vapor or spray. |
|------------------|---|

#### 6.1.1. For non-emergency personnel

|                      |   |
|----------------------|---|
| Emergency procedures | : Only qualified personnel equipped with suitable protective equipment may intervene. |
|----------------------|---|

#### 6.1.2. For emergency responders

|                      |   |
|----------------------|---|
| Protective equipment | : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection". |
| Emergency procedures | : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.   |

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### 6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

### 6.3. Methods and material for containment and cleaning up

- For containment : Stop leak if safe to do so. Dike for recovery or absorb with appropriate material.
- Methods for cleaning up : Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.
- Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

- Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe fumes, mist, spray, vapors. Wear personal protective equipment. Avoid contact with skin and eyes.
- Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

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

- Technical measures : Comply with applicable regulations.
- Storage conditions : Keep container closed when not in use.
- Incompatible materials : Refer to Section 10 on Incompatible Materials.
- Storage temperature : 2 – 8 °C
- Storage area : Store in dry, well-ventilated area.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

| Hexafluoroacetone sesquideuterate (62251-10-9) |  |
|--|--|
| No additional information available            |  |
| Deuterium oxide (7789-20-0)                    |  |
| No additional information available            |  |
| Hexafluoroacetone (684-16-2)                   |  |
| USA - ACGIH - Occupational Exposure Limits     |  |
| Local name                                     | Hexafluoroacetone  |
| ACGIH OEL TWA [ppm]                            | 0.1 ppm  |
| Remark (ACGIH)                                 | Testicular dam; kidney dam   |
| ACGIH chemical category                        | Skin - potential significant contribution to overall exposure by the cutaneous route |
| USA - NIOSH - Occupational Exposure Limits     |  |
| NIOSH REL TWA                                  | 0.7 mg/m <sup>3</sup>  |
| NIOSH REL TWA [ppm]                            | 0.1 ppm  |

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### Hexafluoroacetone (684-16-2)

US-NIOSH chemical category

Potential for dermal absorption

### 8.2. Appropriate engineering controls

Appropriate engineering controls : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

### 8.3. Individual protection measures/Personal protective equipment

#### Hand protection:

protective gloves. 29 CFR 1910.138: Hand Protection

#### Eye protection:

Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection

#### Skin and body protection:

Wear suitable protective clothing

#### Respiratory protection:

In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection

#### Personal protective equipment symbol(s):



#### Other information:

Safety shoes. 29 CFR 1910.136: Foot Protection.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

|   |  |
|---|--|
| Physical state                                  | : Liquid   |
| Color   | : Mixture contains one or more component(s) which have the following colour(s):<br>Colorless |
| Odor  | : Mixture contains one or more component(s) which have the following odour:                  |
| Odor threshold                                  | : No data available  |
| pH  | : No data available  |
| Melting point                                   | : No data available  |
| Freezing point                                  | : No data available  |
| Boiling point                                   | : No data available  |
| Flash point                                     | : No data available  |
| Relative evaporation rate (butyl acetate=1)     | : No data available  |
| Flammability (solid, gas)                       | : No data available  |
| Vapor pressure                                  | : No data available  |
| Relative vapor density at 20 °C                 | : No data available  |
| Relative density                                | : No data available  |
| Solubility                                      | : No data available  |
| Partition coefficient n-octanol/water (Log Pow) | : No data available  |
| Auto-ignition temperature                       | : No data available  |
| Decomposition temperature                       | : No data available  |
| Viscosity, kinematic                            | : No data available  |
| Viscosity, dynamic                              | : No data available  |

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

Explosion limits : No data available  
Explosive properties : No data available  
Oxidizing properties : 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

The product is stable at normal handling and storage conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

Keep away from heat, sparks and flame.

### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity (oral) : Toxic if swallowed.  
Acute toxicity (dermal) : Toxic in contact with skin.  
Acute toxicity (inhalation) : Not classified

| Hexafluoroacetone sesquideuterate (62251-10-9) |                       |
|--|-----------------------|
| ATE US (oral)                                  | 100 mg/kg body weight |
| ATE US (dermal)                                | 300 mg/kg body weight |
| Hexafluoroacetone (684-16-2)                   |                       |
| LC50 Inhalation - Rat [ppm]                    | 300 ppm/4h            |
| ATE US (gases)                                 | 300 ppmV/4h           |

Skin corrosion/irritation : Causes severe skin burns.  
Serious eye damage/irritation : Causes serious eye irritation.  
Respiratory or skin sensitization : Not classified  
Germ cell mutagenicity : Not classified  
Carcinogenicity : Not classified  
Reproductive toxicity : May damage fertility or the unborn child.  
STOT-single exposure : May cause respiratory irritation.

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### Hexafluoroacetone (684-16-2)

|                        |  |
|------------------------|--|
| STOT-single exposure   | May cause respiratory irritation.  |
| STOT-repeated exposure | : Not classified   |
| Aspiration hazard      | : Not classified   |
| Viscosity, kinematic   | : No data available  |
| Symptoms/effects       | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11. |

## 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

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Disposal methods

|  |   |
|--|---|
| Waste treatment methods                    | : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.   |
| Product/Packaging disposal recommendations | : Dispose of contents/container in accordance with licensed collector's sorting instructions. |
| Additional information                     | : Recycle the material as far as possible.  |

## SECTION 14: Transport information

### 14.1. UN number

|               |                  |
|---------------|------------------|
| DOT NA No     | : UN2552         |
| UN-No. (TDG)  | : Not applicable |
| UN-No. (IMDG) | : 2552           |
| UN-No. (IATA) | : 2552           |

### 14.2. UN proper shipping name

|                             |                                     |
|-----------------------------|-------------------------------------|
| Proper Shipping Name (DOT)  | : Hexafluoroacetone hydrate, liquid |
| Proper Shipping Name (TDG)  | : Not applicable                    |
| Proper Shipping Name (IMDG) | : HEXAFLUOROACETONE HYDRATE, LIQUID |
| Proper Shipping Name (IATA) | : Hexafluoroacetone hydrate, liquid |

### 14.3. Transport hazard class(es)

#### DOT

|                                  |       |
|----------------------------------|-------|
| Transport hazard class(es) (DOT) | : 6.1 |
|----------------------------------|-------|

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

Hazard labels (DOT) : 6.1



### TDG

Transport hazard class(es) (TDG) : Not applicable

### IMDG

Transport hazard class(es) (IMDG) : 6.1

Hazard labels (IMDG) : 6.1



### IATA

Transport hazard class(es) (IATA) : 6.1

Hazard labels (IATA) : 6.1



## 14.4. Packing group

Packing group (DOT) : II

Packing group (TDG) : Not applicable

Packing group (IMDG) : II

Packing group (IATA) : II

## 14.5. Environmental hazards

Other information : No supplementary information available.

## 14.6. Special precautions for user

### DOT

UN-No.(DOT) : UN2552

DOT Special Provisions (49 CFR 172.102) : IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized.

T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3)

TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.

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

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

|  |   |
|--|---|
| DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) | : 5 L   |
| DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)     | : 60 L  |
| 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"  |

### TDG

Emergency Response Guide (ERG) Number : 151

### IMDG

|                                    |   |
|------------------------------------|---|
| Limited quantities (IMDG)          | : 100 ml  |
| Excepted quantities (IMDG)         | : E4  |
| Packing instructions (IMDG)        | : P001  |
| IBC packing instructions (IMDG)    | : IBC02   |
| Tank instructions (IMDG)           | : T7  |
| Tank special provisions (IMDG)     | : TP2   |
| EmS-No. (Fire)                     | : F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE      |
| EmS-No. (Spillage)                 | : S-A - SPILLAGE SCHEDULE Alfa - TOXIC SUBSTANCES       |
| Stowage category (IMDG)            | : B   |
| Stowage and handling (IMDG)        | : SW2   |
| Properties and observations (IMDG) | : Toxic if swallowed, by skin contact or by inhalation. |

### IATA

|  |        |
|--|--------|
| PCA Excepted quantities (IATA)               | : E4   |
| PCA Limited quantities (IATA)                | : Y641 |
| PCA limited quantity max net quantity (IATA) | : 1L   |
| PCA packing instructions (IATA)              | : 654  |
| PCA max net quantity (IATA)                  | : 5L   |
| CAO packing instructions (IATA)              | : 662  |
| CAO max net quantity (IATA)                  | : 60L  |
| ERG code (IATA)                              | : 6L   |

### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

### 15.2. International regulations

#### CANADA

##### Deuterium oxide (7789-20-0)

Listed on the Canadian DSL (Domestic Substances List)

##### Hexafluoroacetone (684-16-2)

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

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

### EU-Regulations

#### Deuterium oxide (7789-20-0)

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

#### Hexafluoroacetone (684-16-2)

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

### National regulations

#### Deuterium oxide (7789-20-0)

Listed introduction on Australian Industrial Chemicals Introduction Scheme (AICIS Inventory)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Listed on KECL/KECI (Korean Existing Chemicals Inventory)  
Listed on NZIoC (New Zealand Inventory of Chemicals)

#### Hexafluoroacetone (684-16-2)

Listed on the Japanese ENCS (Existing New Chemical Substances) inventory  
Listed on KECL/KECI (Korean Existing Chemicals Inventory)  
Listed on NZIoC (New Zealand Inventory of Chemicals)  
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)  
Listed on INSQ (Mexican National Inventory of Chemical Substances)

### 15.3. US State regulations



#### WARNING:

This product can expose you to Hexafluoroacetone, which is known to the State of California to cause birth defects or other reproductive harm. For more information go to [www.P65Warnings.ca.gov](http://www.P65Warnings.ca.gov).

| Component                   | State or local regulations  |
|-----------------------------|---|
| Hexafluoroacetone(684-16-2) | U.S. - Massachusetts - Right To Know List; U.S. - New Jersey - Right to Know Hazardous Substance List; U.S. - Pennsylvania - RTK (Right to Know) List |

## SECTION 16: Other information

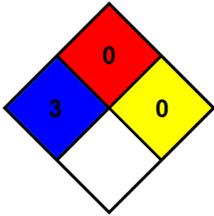
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| Full text of H-phrases |  |
|------------------------|--|
| H280                   | Contains gas under pressure; may explode if heated |
| H301                   | Toxic if swallowed                                 |
| H311                   | Toxic in contact with skin                         |
| H314                   | Causes severe skin burns and eye damage            |
| H318                   | Causes serious eye damage                          |
| H319                   | Causes serious eye irritation                      |
| H330                   | Fatal if inhaled                                   |
| H335                   | May cause respiratory irritation                   |
| H360                   | May damage fertility or the unborn child           |

# Hexafluoroacetone sesquideuterate

## Safety Data Sheet

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

|                    |   |   |
|--------------------|---|---|
| NFPA health hazard | : 3 - Materials that, under emergency conditions, can cause serious or permanent injury.  |  |
| NFPA fire hazard   | : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.                               |   |
| NFPA reactivity    | : 0 - Material that in themselves are normally stable, even under fire conditions.  |   |
| Hazard Rating      |   |   |
| Health             | : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given   |   |
| Flammability       | : 0 Minimal Hazard - Materials that will not burn   |   |
| 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. |   |

Safety Data Sheet (SDS), USA

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 offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.