

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: Thiophenol
CAS No	: 108-98-5
Product code	: 5661-1-X0
Formula	: C6H6S
Synonyms	: Benzenethiol; Phenyl mercaptan
Other means of identification	: MFCD00004826

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

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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1.3. Details of the supplier of the safety data sheet

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

Classification (GHS-US)

Flam. Liq. 3	H226 - Flammable liquid and vapour
Acute Tox. 1 (Oral)	H300 - Fatal if swallowed
Acute Tox. 2 (Dermal)	H310 - Fatal in contact with skin
Acute Tox. 2 (Inhalation)	H330 - Fatal if inhaled
Skin Irrit. 2	H315 - Causes skin irritation
Eye Dam. 1	H318 - Causes serious eye damage
Repr. 2	H361 - Suspected of damaging fertility or the unborn child
STOT SE 3	H335 - May cause respiratory irritation
STOT RE 1	H372 - Causes damage to organs through prolonged or repeated exposure
Aquatic Acute 1	H400 - Very toxic to aquatic life
Aquatic Chronic 1	H410 - Very toxic to aquatic life with long lasting effects

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS02

GHS05

GHS06

GHS07

GHS08

GHS09

Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H226 - Flammable liquid and vapor
H300+H310+H330 - Fatal if swallowed, in contact with skin or if inhaled
H315 - Causes skin irritation
H318 - Causes serious eye damage
H335 - May cause respiratory irritation
H361 - Suspected of damaging fertility or the unborn child
H372 - Causes damage to organs through prolonged or repeated exposure
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use
P202 - Do not handle until all safety precautions have been read and understood
P210 - Keep away from heat/sparks/open flames/hot surfaces. No smoking

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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 fumes, mist, spray, vapors
P262 - Do not get in eyes, on skin, or on clothing
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
P273 - Avoid release to the environment
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P284 - In case of inadequate ventilation wear respiratory protection
P301+P310 - If swallowed: Immediately call a poison center/doctor/...
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
P314 - Get medical advice/attention if you feel unwell
P320 - Specific treatment is urgent (see supplemental first aid instructions on this label)
P321 - Specific treatment (see supplemental first aid instructions on this label)
P330 - Rinse mouth
P332+P313 - If skin irritation occurs: Get medical advice/attention
P361 - Take off immediately all contaminated clothing
P362+P364 - Take off contaminated clothing and wash it before reuse
P363 - Wash contaminated clothing before reuse
P370+P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
P391 - Collect spillage
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. Other hazards

Other hazards not contributing to the classification : Stench.

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/information on ingredients

3.1. Substance

Substance type : Mono-constituent

Name	Product identifier	%	Classification (GHS-US)
Thiophenol (Main constituent)	(CAS No) 108-98-5	<= 100	Flam. Liq. 3, H226 Acute Tox. 1 (Oral), H300 Acute Tox. 2 (Dermal), H310 Acute Tox. 2 (Inhalation), H330 Skin Irrit. 2, H315 Eye Dam. 1, H318 Repr. 2, H361 STOT SE 3, H335 STOT RE 1, H372 Aquatic Acute 1, H400 Aquatic Chronic 1, H410

Full text of H-phrases: see section 16

3.2. Mixture

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.

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| 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, both acute and delayed

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| Symptoms/injuries | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11. |
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4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

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| Suitable extinguishing media | : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire. |
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5.2. Special hazards arising from the substance or mixture

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| Fire hazard | : Thermal decomposition generates: Carbon oxides. Sulfur oxides. |
| Explosion hazard | : Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers. May form flammable/explosive vapor-air mixture. |

5.3. Advice for firefighters

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| Firefighting instructions | : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion. |
| 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

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

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| Emergency procedures | : Only qualified personnel equipped with suitable protective equipment may intervene. |
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6.1.2. For emergency responders

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|----------------------|--|
| 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. Consider the risk of potentially explosive atmospheres. Eliminate every possible source of ignition. |

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

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|-------------------------|---|
| 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

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| Additional hazards when processed | : Handle empty containers with care because residual vapors are flammable. |
| 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. Keep away from ignition sources (including static discharges). Proper grounding procedures to avoid static electricity should be followed. Use only non-sparking tools. |

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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. Keep away from ignition sources. Air sensitive. Keep contents under inert gas.
Incompatible materials : Refer to Section 10 on Incompatible Materials.
Prohibitions on mixed storage : Do not store with: Acids.
Storage area : Store in dry, cool, well-ventilated area.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Thiophenol (108-98-5)		
ACGIH	ACGIH TWA (ppm)	0.10 ppm
ACGIH	Remark (ACGIH)	CNS impair; eye & skin irr

8.2. Exposure 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.
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.
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
Appearance : Water-white liquid.
Color : white
Odor : penetrating very strong garlic-like Lachrymator
Odor threshold : No data available
pH : No data available
Melting point : -15 °C
Freezing point : No data available
Boiling point : 169 °C
Flash point : 50 °C
Relative evaporation rate (butyl acetate=1) : No data available
Flammability (solid, gas) : No data available
Explosion limits : No data available
Explosive properties : No data available
Oxidizing properties : No data available
Vapor pressure : 1.4 mm Hg (@ 20 °C)
Relative density : No data available
Relative vapor density at 20 °C : No data available
Specific gravity / density : 1.0726 g/ml (@ 25 °C)
Molecular mass : 110.177 g/mol
Solubility : No data available
Log Pow : 2.52
Auto-ignition temperature : No data available
Decomposition temperature : No data available
Viscosity : No data available
Viscosity, kinematic : No data available

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Viscosity, dynamic : No data available

9.2. Other information

Refractive index : 1.588 (@ 20 °C)

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

Acids. Strong bases. 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: Fatal if swallowed. Dermal: Fatal in contact with skin. Inhalation: Fatal if inhaled.

Thiophenol (108-98-5)	
LD50 oral rat	46 mg/kg
LD50 dermal rabbit	134 mg/kg
LC50 inhalation rat (ppm)	33 ppm/4h
ATE US (oral)	0.500 mg/kg body weight
ATE US (dermal)	134.000 mg/kg body weight
ATE US (gases)	33.000 ppmV/4h
ATE US (vapors)	0.500 mg/l/4h
ATE US (dust, mist)	0.050 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.

Serious eye damage/irritation : Causes serious eye damage.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

Reproductive toxicity : Suspected of damaging fertility or the unborn child.

Specific target organ toxicity (single exposure) : May cause respiratory irritation.

Specific target organ toxicity (repeated exposure) : Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard : Not classified

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Thiophenol (108-98-5)	
Log Pow	2.52

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12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

- Regional legislation (waste) : U.S. - RCRA (Resource Conservation & Recovery Act) - Hazardous Constituents - Appendix VIII to 40 CFR 261. U.S. - RCRA (Resource Conservation & Recovery Act) - P Series Wastes - Acutely Toxic Wastes.
- Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
- Waste 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

Department of Transportation (DOT)

In accordance with DOT

- Transport document description : UN2337 Phenyl mercaptan, 6.1, I
- UN-No.(DOT) : UN2337
- Proper Shipping Name (DOT) : Phenyl mercaptan
- Transport hazard class(es) (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132
- Hazard labels (DOT) : 6.1 - Poison
3 - Flammable liquid



- Packing group (DOT) : I - Great Danger
- Dangerous for the environment : Yes
- Marine pollutant : Yes



- DOT Packaging Non Bulk (49 CFR 173.xxx) : 227
- DOT Packaging Bulk (49 CFR 173.xxx) : 244

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- DOT Special Provisions (49 CFR 172.102) : 2 - This material is poisonous by inhalation (see 171.8 of this subchapter) in Hazard Zone B (see 173.116(a) or 173.133(a) of this subchapter), and must be described as an inhalation hazard under the provisions of this subchapter.
B9 - Bottom outlets are not authorized.
B14 - Each bulk packaging, except a tank car or a multi-unit-tank car tank, must be insulated with an insulating material so that the overall thermal conductance at 15.5 C (60 F) is no more than 1.5333 kilojoules per hour per square meter per degree Celsius (0.075 Btu per hour per square foot per degree Fahrenheit) temperature differential. Insulating materials must not promote corrosion to steel when wet.
B32 - MC 312, MC 330, MC 331, DOT 412 cargo tanks and DOT 51 portable tanks must be made of stainless steel, except that steel other than stainless steel may be used in accordance with the provisions of 173.24b(b) of this subchapter. Thickness of stainless steel for tank shell and heads for cargo tanks and portable tanks must be the greater of 6.35 mm (0.250 inch) or the thickness required for a tank with a design pressure at least equal to 1.3 times the vapor pressure of the lading at 46 C (115 F). In addition, MC 312 and DOT 412 cargo tank motor vehicles must: a. Be ASME Code (U) stamped for 100% radiography of all pressure-retaining welds; b. Have accident damage protection which conforms with 178.3458 of this subchapter; c. Have a MAWP or design pressure of at least 87 psig; and d. Have a bolted man way cover.
B77 - Other packaging are authorized when approved by the Associate Administrator.
T20 - 10 8 mm Prohibited 178.275(g)(3).
TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: t_r is the maximum mean bulk temperature during transport, t_f 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 (t_f) and the maximum mean bulk temperature during transportation (t_r) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d_{15} and d_{50} are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
TP13 - Self-contained breathing apparatus must be provided when this hazardous material is transported by sea.
TP38 - Each portable tank must be insulated with an insulating material so that the overall thermal conductance at 15.5 C (60 F) is no more than 1.5333 kilojoules per hour per square meter per degree Celsius (0.075 Btu per hour per square foot per degree Fahrenheit) temperature differential. Insulating materials may not promote corrosion to steel when wet.
TP45 - Each portable tank must be made of stainless steel, except that steel other than stainless steel may be used in accordance with the provisions of 173.24b(b) of this subchapter. Thickness of stainless steel for portable tank shells and heads must be the greater of 6.35 mm (0.250 inch) or the thickness required for a portable tank with a design pressure at least equal to 1.3 times the vapor pressure of the hazardous material at 46 C (115 F).
- DOT Packaging Exceptions (49 CFR 173.xxx) : None
- DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : Forbidden
- DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : Forbidden
- DOT Vessel Stowage Location : D - The material must be stowed "on deck only" 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, but the material is prohibited on passenger vessels in which the limiting number of passengers is exceeded.
- DOT Vessel Stowage Other : 40 - Stow "clear of living quarters", 52 - Stow "separated from" acids
- Emergency Response Guide (ERG) Number : 131
- Other information : No supplementary information available.

TDG

No additional information available

Transport by sea

- UN-No. (IMDG) : 2337
- Proper Shipping Name (IMDG) : PHENYL MERCAPTAN
- Class (IMDG) : 6.1 - Toxic substances
- Packing group (IMDG) : I - substances presenting high danger

Air transport

- UN-No. (IATA) : 2337
- Proper Shipping Name (IATA) : Phenyl mercaptan
- Class (IATA) : 6.1 - Toxic Substances

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SECTION 15: Regulatory information

15.1. US Federal regulations

Thiophenol (108-98-5)

Listed on the United States TSCA (Toxic Substances Control Act) inventory
Listed on the United States SARA Section 302

CERCLA RQ	100 lb
SARA Section 302 Threshold Planning Quantity (TPQ)	500 lb

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

This product or mixture does not contain a toxic chemical or chemicals in excess of the applicable de minimis concentration as specified in 40 CFR §372.38(a) subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR Part 372.

15.2. International regulations

CANADA

Thiophenol (108-98-5)

Listed on the Canadian DSL (Domestic Substances List)

WHMIS Classification	Class B Division 3 - Combustible Liquid Class D Division 1 Subdivision A - Very toxic material causing immediate and serious toxic effects Class D Division 2 Subdivision B - Toxic material causing other toxic effects
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EU-Regulations

No additional information available

National regulations

Thiophenol (108-98-5)

Listed on the AICS (Australian Inventory of Chemical Substances)
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)
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
Japanese Pollutant Release and Transfer Register Law (PRTR Law)
Listed on the Canadian IDL (Ingredient Disclosure List)
Listed on INSQ (Mexican national Inventory of Chemical Substances)
Listed on the TCSI (Taiwan Chemical Substance Inventory)

15.3. US State regulations

Thiophenol (108-98-5)

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List U.S. - Pennsylvania - RTK (Right to Know) List
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California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer and/or reproductive harm

SECTION 16: Other information

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Full text of H-phrases:

Acute Tox. 1 (Oral)	Acute toxicity (oral) Category 1
Acute Tox. 2 (Dermal)	Acute toxicity (dermal) Category 2
Acute Tox. 2 (Inhalation)	Acute toxicity (inhalation) Category 2
Aquatic Acute 1	Hazardous to the aquatic environment - Acute Hazard Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment - Chronic Hazard Category 1
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Flam. Liq. 3	Flammable liquids Category 3
Repr. 2	Reproductive toxicity Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT RE 1	Specific target organ toxicity (repeated exposure) Category 1
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H226	Flammable liquid and vapor
H300	Fatal if swallowed
H310	Fatal in contact with skin
H315	Causes skin irritation
H318	Causes serious eye damage
H330	Fatal if inhaled
H335	May cause respiratory irritation
H361	Suspected of damaging fertility or the unborn child
H372	Causes damage to organs through prolonged or repeated exposure
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

NFPA health hazard

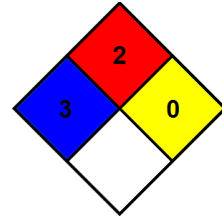
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard

: 2 - Must be moderately heated or exposed to relatively high temperature before ignition can occur.

NFPA reactivity

: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health : 4 Severe Hazard - Life-threatening, major or permanent damage may result from single or repeated overexposures

* - Chronic (long-term) health effects may result from repeated overexposure

Flammability

: 2 Moderate Hazard - Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F. (Classes II & IIIA)

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.

SDS US (GHS HazCom 2012)

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.