

4-(Pentafluorothio)benzotrile

Safety Data Sheet 76713X1

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

Date of issue: 09/14/2018

Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: 4-(Pentafluorothio)benzotrile
CAS No	: 401892-85-1
Product code	: 7671-3-X1
Formula	: C7H4F5NS
Synonyms	: 4-Cyanophenylsulfur pentafluoride; 4-(Pentafluorosulfanyl)benzotrile
Other means of identification	: MFCD03788521

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)

Acute Tox. 4 (Oral)	H302 - Harmful if swallowed
Acute Tox. 4 (Dermal)	H312 - Harmful in contact with skin
Acute Tox. 4 (Inhalation)	H332 - Harmful if inhaled
Skin Irrit. 2	H315 - Causes skin irritation
Eye Irrit. 2A	H319 - Causes serious eye irritation
STOT SE 3	H335 - May cause respiratory irritation

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H302+H312+H332 - Harmful if swallowed, in contact with skin or if inhaled
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P261 - Avoid breathing dust, mist, 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+P312 - If swallowed: Call a POISON CENTER or doctor/ physician if you feel unwell
P302+P352 - If on skin: Wash with plenty of soap and water
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P312 - Call a POISON CENTER or doctor/physician if you feel unwell
P321 - Specific treatment (see supplemental first aid instructions on this label)

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P330 - Rinse mouth
P332+P313 - If skin irritation occurs: Get medical advice/attention
P337+P313 - If eye irritation persists: Get medical advice/attention
P362+P364 - Take off contaminated clothing and wash it 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

No additional information available

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)
4-(Pentafluorothio)benzotrile (Main constituent)	(CAS No) 401892-85-1	<= 100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

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.

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

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

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

Treat symptomatically.

SECTION 5: Firefighting measures

5.1. Extinguishing media

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

5.2. Special hazards arising from the substance or mixture

Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. Nitrogen oxides. Sulfur oxides.

5.3. Advice for firefighters

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 dust.

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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".

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.
Methods for cleaning up : Sweep or shovel spills into appropriate container for disposal. Minimize generation of dust.
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 dust, mist, spray. 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. Keep away from ignition sources. Air sensitive. Keep contents under inert gas.
Incompatible materials : Refer to Section 10 on Incompatible Materials.
Storage area : Store in dry, cool, well-ventilated area.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

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 : Solid
Color : No data available
Odor : No data available
Odor threshold : No data available
pH : No data available
Melting point : 102 - 105 °C
Freezing point : No data available
Boiling point : No data available
Flash point : No data available
Relative evaporation rate (butyl acetate=1) : No data available

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Flammability (solid, gas)	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Vapor pressure	: No data available
Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Molecular mass	: 229.17 g/mol
Solubility	: No data available
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: 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: Harmful if swallowed. Dermal: Harmful in contact with skin. Inhalation: Harmful if inhaled.
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

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

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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. Waste treatment methods

- 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 : UN2811 Toxic solids, organic, n.o.s., 6.1, III
UN-No.(DOT) : UN2811
Proper Shipping Name (DOT) : Toxic solids, organic, n.o.s.
Transport hazard class(es) (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132
Hazard labels (DOT) : 6.1 - Poison



- Packing group (DOT) : III - Minor Danger
DOT Packaging Non Bulk (49 CFR 173.xxx) : 213
DOT Packaging Bulk (49 CFR 173.xxx) : 240
DOT Symbols : G - Identifies PSN requiring a technical name
DOT Special Provisions (49 CFR 172.102) : IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2).
IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner.
T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2)
TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
DOT Packaging Exceptions (49 CFR 173.xxx) : 153
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 100 kg
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 200 kg
DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

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Other information : No supplementary information available.

TDG

No additional information available

Transport by sea

UN-No. (IMDG) : 2811
Proper Shipping Name (IMDG) : TOXIC SOLID, ORGANIC, N.O.S.
Class (IMDG) : 6.1 - Toxic substances
Packing group (IMDG) : III - substances presenting low danger

Air transport

UN-No. (IATA) : 2811
Proper Shipping Name (IATA) : Toxic solid, organic, n.o.s.
Class (IATA) : 6.1 - Toxic Substances
Packing group (IATA) : III - Minor Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

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

4-(Pentafluorothio)benzotrile	CAS No 401892-85-1	100%
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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

No additional information available

EU-Regulations

No additional information available

National regulations

No additional information available

15.3. US State regulations

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

Full text of H-phrases:

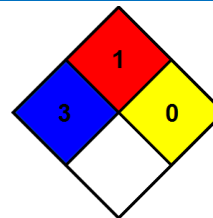
Acute Tox. 4 (Dermal)	Acute toxicity (dermal) Category 4
Acute Tox. 4 (Inhalation)	Acute toxicity (inhalation) Category 4
Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
H335	May cause respiratory irritation

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- NFPA health hazard : 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.
- NFPA fire hazard : 1 - Must be preheated before ignition can occur.
- NFPA reactivity : 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

- Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
- Flammability : 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB)
- 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.