Heptafluoroisobutyronitrile

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
SDS ID: 3137201
Issue date: 11/4/2022 Revision date: 4/30/2025 Version: 1.2

SECTION 1: Identification

1.1. Identification

Product form	:	Substance
Substance name	:	Heptafluoroisobutyronitrile
CAS-No.	:	42532-60-5
Product code	:	3137-2-01
Formula	:	C4F7N
Synonyms	:	2,3,3,3-Tetrafluoro-2-(trifluoromethyl)propanenitrile
Other means of identification	:	MFCD18641876

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.
P.O. Box 309
Alachua, FL, Alachua, 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

GHS US classification

Gases under pressure Liquefied gas	H280	Contains gas under pressure; may explode if heated
Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Acute toxicity (inhalation:gas) Category 4	H332	Harmful if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation
Simple Asphyxiant	SIAS	May displace oxygen and cause rapid suffocation

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) : Warning

Hazard statements (GHS US) : H280 - Contains gas under pressure; may explode if heated
H302+H332 - Harmful if swallowed or if inhaled
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
May displace oxygen and cause rapid suffocation

Precautionary statements (GHS US) : P261 - Avoid breathing 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+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)
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.
P410+P403 - Protect from sunlight. Store in a well-ventilated place.
P501 - Dispose of contents/container to an approved waste disposal plant

2.3. Other hazards which do not result in classification

Other hazards which do not result in classification : May cause frostbite. Risk of explosion if heated under confinement.

2.4. Unknown acute toxicity (GHS US)

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
Heptafluoroisobutyronitrile (Main constituent)	CAS-No.: 42532-60-5	≤ 100	Press. Gas (Liq.), H280 Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Inhalation:gas), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335 Simple Asphy, SIAS

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

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 : Thaw frosted parts with lukewarm water. Do not rub affected area. Get immediate medical advice/attention.

First-aid measures after eye contact : Remove contact lenses, if present and easy to do. Continue rinsing. Immediately flush eyes thoroughly with water for at least 15 minutes. Get immediate medical advice/attention.

First-aid measures after ingestion : Due to its physical form, exposure to this chemical is not likely. 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.

Symptoms/effects after inhalation : May cause drowsiness or dizziness.

Symptoms/effects after skin contact : Contact with the liquid the may cause cold burns/frostbite.

Symptoms/effects after eye contact : Direct contact with the liquefied gas may cause severe and possibly permanent eye injury due to frostbite from rapid liquid evaporation.

4.3. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

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. Nitrogen oxides.

Explosion hazard : Contains gas under pressure; may explode if heated. Use water spray or fog for cooling exposed containers.

5.3. Special protective equipment and precautions for fire-fighters

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

General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. May cause suffocation by reducing oxygen available for breathing. 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.

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	:	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

Additional hazards when processed	:	Pressurized container: Do not pierce or burn, even after use. Close valve after each use and when empty.
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, gas, 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	:	Protect from sunlight. Do not expose to temperatures exceeding 50 °C. Keep container closed when not in use.
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. 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. Systems under pressure should be regularly checked for leakage. Oxygen detectors should be used when asphyxiating gases may be released. Gas detectors should be used when toxic gases may be released.

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):

Thermal hazard protection:

Cold insulating gloves.

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	:	Gas
Color	:	No data available
Odor	:	No data available
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
Molecular mass	:	195.0383 g/mol
Solubility	:	No data available
Partition coefficient n-octanol/water (Log Pow)	:	4.3 (at 24 °C)
Auto-ignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity, kinematic	:	No data available
Viscosity, dynamic	:	No data available
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 acids. Strong bases. Strong oxidizing agents. Strong reducing 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.
Acute toxicity (dermal) : Not classified
Acute toxicity (inhalation) : Inhalation:gas: Harmful if inhaled.

Heptafluoroisobutyronitrile (42532-60-5)	
LC50 Inhalation - Rat [ppm]	15000 ppm/4h
ATE US (gases)	15000 ppmV/4h

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
STOT-single exposure : May cause respiratory irritation.
STOT-repeated exposure : Not classified
Aspiration hazard : Not applicable
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.
Symptoms/effects after inhalation : May cause drowsiness or dizziness.
Symptoms/effects after skin contact : Contact with the liquid the may cause cold burns/frostbite.
Symptoms/effects after eye contact : Direct contact with the liquefied gas may cause severe and possibly permanent eye injury due to frostbite from rapid liquid evaporation.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

Heptafluoroisobutyronitrile (42532-60-5)	
Persistence and degradability	Not readily biodegradable. May cause long-term adverse effects in the environment. PBT - Persistent, Bioaccumulative and Toxic.

12.3. Bioaccumulative potential

Heptafluoroisobutyronitrile (42532-60-5)	
Partition coefficient n-octanol/water (Log Pow)	4.3 (at 24 °C)
Bioaccumulative potential	Perfluorinated alkanes (PFAs, “forever chemicals”) are long lasting, widely used chemicals that break down slowly over time. The potential hazards of PFAs are under investigation and have not been established.

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.

Sewage disposal recommendations : See the EPA's Interim Guidance on PFAS Destruction and Disposal.

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.

Ecological information : This material is considered to be a “Forever chemical”. Prevent any possible release to the environment. Do not discharge into drains. Take all necessary measures to prevent accidental discharge of products into drains and waterways due to the rupture of containers or transfer systems, or emergency response.

SECTION 14: Transport information

14.1. UN number

DOT NA No : UN3163

UN-No. (TDG) : UN3163

UN-No. (IMDG) : 3163

UN-No. (IATA) : 3163

14.2. UN proper shipping name

Proper Shipping Name (DOT) : Liquefied gas, n.o.s.

Proper Shipping Name (TDG) : LIQUEFIED GAS, N.O.S.

Proper Shipping Name (IMDG) : LIQUEFIED GAS, N.O.S.

Proper Shipping Name (IATA) : Liquefied gas, n.o.s.

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT) : 2.2

Hazard labels (DOT) : 2.2

TDG

Transport hazard class(es) (TDG) : 2.2

Hazard labels (TDG) : 2.2

IMDG

Transport hazard class(es) (IMDG) : 2.2

Hazard labels (IMDG) : 2.2

IATA

Transport hazard class(es) (IATA) : 2.2

Hazard labels (IATA) : 2.2

14.4. Packing group

Packing group (DOT) : Not applicable

Packing group (TDG) : Not applicable

Packing group (IMDG) : Not applicable

Packing group (IATA) : Not applicable

14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

DOT

UN-No.(DOT) : UN3163

DOT Special Provisions (49 CFR 172.102) : T50 - When portable tank instruction T50 is referenced in Column (7) of the 172.101 Table, the applicable liquefied compressed gases are authorized to be transported in portable tanks in accordance with the requirements of 173.313 of this subchapter.

DOT Packaging Exceptions (49 CFR 173.xxx) : 306

DOT Packaging Non Bulk (49 CFR 173.xxx) : 304

DOT Packaging Bulk (49 CFR 173.xxx) : 314, 315

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 75 kg

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	:	150 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.

TDG

UN-No. (TDG)	:	UN3163
TDG Special Provisions	:	16 - 1) The technical name of the most dangerous substance related to the primary class must be shown, in parentheses, on the shipping document following the shipping name in accordance with clause 3.5(1)(c)(i)(A) of Part 3, Documentation. The technical name must also be shown, in parentheses, on a small means of containment or on a tag following the shipping name in accordance with subsections 4.11(2) and (3) of Part 4, Dangerous Goods Safety Marks. 2) subsection (1), the technical name for the following dangerous goods is not required to be shown on a shipping document or on a small means of containment when Canadian law for domestic transport or an international convention for international transport prohibits the disclosure of the technical: a) UN1544, ALKALOID SALTS, SOLID, N.O.S. or ALKALOIDS, SOLID, N.O.S; b) UN1851, MEDICINE, LIQUID, TOXIC, N.O.S; c) UN3140, ALKALOID SALTS, LIQUID, N.O.S. or ALKALOIDS, LIQUID, N.O.S; d) UN3248, MEDICINE, LIQUID, FLAMMABLE, TOXIC, N.O.S; or e) UN3249, MEDICINE, SOLID, TOXIC, N.O.S. An example in Canada is the “Food and Drugs Act”.
Explosive Limit and Limited Quantity Index	:	0.125 L
Excepted quantities (TDG)	:	E1
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	:	75 L
Emergency Response Guide (ERG) Number	:	126

IMDG

Special provision (IMDG)	:	274
Limited quantities (IMDG)	:	120 ml
Excepted quantities (IMDG)	:	E1
Packing instructions (IMDG)	:	P200
Tank instructions (IMDG)	:	T50
EmS-No. (Fire)	:	F-C - FIRE SCHEDULE Charlie - NON-FLAMMABLE GASES
EmS-No. (Spillage)	:	S-V - SPILLAGE SCHEDULE Victor - GASES (NON-FLAMMABLE, NON-TOXIC)
Stowage category (IMDG)	:	A

IATA

PCA Excepted quantities (IATA)	:	E1
PCA Limited quantities (IATA)	:	Forbidden
PCA limited quantity max net quantity (IATA)	:	Forbidden
PCA packing instructions (IATA)	:	200
PCA max net quantity (IATA)	:	75kg
CAO packing instructions (IATA)	:	200
CAO max net quantity (IATA)	:	150kg
ERG code (IATA)	:	2L

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

No additional information available

EU-Regulations

No additional information available

National regulations

Heptafluoroisobutyronitrile (42532-60-5)
Listed on NZIoC (New Zealand Inventory of Chemicals) Listed on the Japanese ISHL (Industrial Safety and Health Law)

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

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

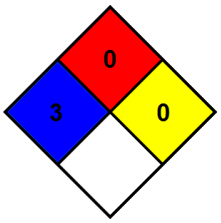
Revision date : 4/30/2025

Full text of H-phrases	
H280	Contains gas under pressure; may explode if heated
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
H335	May cause respiratory irritation

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.