

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations SDS ID: 6164326

Issue date: 07.03.2018 Revision date: 18.12.2023 Version: 1.1

SECTION 1: Identification

1.1. Identification

Product form : Substance

Substance name : 1H,1H-Heptafluorobutyl trifluoromethanesulfonate

CAS-No. : 6401-01-0
Product code : 6164-3-26
Formula : C5H2F10O3S

Synonyms : 1H,1H-Heptafluorobutyl triflate

Other means of identification : MFCD02093339

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 - 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

H301 Acute toxicity (oral) Category 3 Toxic if swallowed Acute toxicity (dermal) Category 3 H311 Toxic in contact with skin Acute toxicity (inhalation) Category 3 Toxic if inhaled H331 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, H335 May cause respiratory irritation

Respiratory tract 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+H331 - Toxic if swallowed, in contact with skin or if inhaled

H315 - Causes skin irritation

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Precautionary statements (GHS US)

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H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

: P261 - Avoid breathing fumes, mist, spray, vapors.

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.

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.

P311 - Call a POISON CENTER or doctor/physician

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.

P361 - Take off immediately all contaminated clothing.

P362+P364 - Take off 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)

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
1H,1H-Heptafluorobutyl trifluoromethanesulfonate (Main constituent)	CAS-No.: 6401-01-0	≤ 100	Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Inhalation), H331 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

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

3.2. Mixtures

Not applicable

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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. Remove contaminated clothing and shoes. 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.

Symptoms/effects after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

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. Sulfur oxides.

Explosion hazard : Risk of explosion if heated under confinement. 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. 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".

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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. 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. Moisture 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

1H,1H-Heptafluorobutyl trifluoromethanesulfonate (6401-01-0)

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.

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

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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 : 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 : 118 – 120 °C (@ 732 mm Hg)

Flash point : No data available : No data available Relative evaporation rate (butyl acetate=1) 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 332,117 g/mol 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 **Explosion limits** : No data available Explosive properties : No data available

9.2. Other information

Oxidizing properties

Refractive index : 1,302 (@ 25 °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.

No data available

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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) : Toxic if inhaled.

1H,1H-Heptafluorobutyl trifluoromethanesulfonate (6401-01-0)		
ATE US (oral)	100 mg/kg body weight	
ATE US (dermal)	300 mg/kg body weight	
ATE US (gases)	700 ppmV/4h	
ATE US (vapors)	3 mg/l/4h	
ATE US (dust, mist)	0,5 mg/l/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 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.

Symptoms/effects after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough,

shortness of breath, headache, nausea.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

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12.2. Persistence and degradability

1H,1H-Heptafluorobutyl trifluoromethanesulfonate (6401-01-0)

Persistence and degradability

Not readily biodegradable. May cause long-term adverse effects in the environment. PBT -

Persistent, Bioaccumulative and Toxic.

12.3. Bioaccumulative potential

1H,1H-Heptafluorobutyl trifluoromethanesulfonate (6401-01-0)

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

Sewage disposal recommendations

Product/Packaging disposal recommendations

Additional information

Ecology - waste materials

- : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
- : See the EPA's Interim Guidance on PFAS Destruction and Disposal.
- : Dispose of contents/container in accordance with licensed collector's sorting instructions.
- : Recycle the material as far as possible.

: 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 : UN2927 UN-No. (TDG) : Not applicable

UN-No. (IMDG) : 2927 UN-No. (IATA) : 2927

14.2. UN proper shipping name

Proper Shipping Name (DOT) : Toxic liquids, corrosive, organic, n.o.s.

Proper Shipping Name (TDG) : Not applicable

Proper Shipping Name (IMDG) : TOXIC LIQUID, CORROSIVE, ORGANIC, N.O.S.

Proper Shipping Name (IATA) : Toxic liquid, corrosive, organic, n.o.s.

14.3. Transport hazard class(es)

DOT

Transport hazard class(es) (DOT) : 6.1 (8) Hazard labels (DOT) : 6.1, 8

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TDG

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

IMDG

Transport hazard class(es) (IMDG) : 6.1 (8) Hazard labels (IMDG) : 6.1, 8





ΙΔΤΔ

Transport hazard class(es) (IATA) : 6.1 (8) Hazard labels (IATA) : 6.1, 8





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) : UN2927

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.

T11 - 6 178.274(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.

TP27 - A portable tank having a minimum test pressure of 4 bar (400 kPa) may be used provided the calculated test pressure is 4 bar or less based on the MAWP of the hazardous material, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.

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

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DOT Quantity Limitations Passenger aircraft/rail (49 : 1 L

CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 30 L

CFR 175.75)

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

No data available

IMDG

Special provision (IMDG) : 274
Limited quantities (IMDG) : 100 ml
Excepted quantities (IMDG) : E4
Packing instructions (IMDG) : P001
IBC packing instructions (IMDG) : IBC02
Tank instructions (IMDG) : T11
Tank special provisions (IMDG) : TP2, TP27

EmS-No. (Fire) : F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE EmS-No. (Spillage) : S-B - SPILLAGE SCHEDULE Bravo - CORROSIVE SUBSTANCES

Stowage category (IMDG) : B

IATA

PCA Excepted quantities (IATA) : E4 PCA Limited quantities (IATA) : Y640 PCA limited quantity max net quantity (IATA) : 0.5L PCA packing instructions (IATA) 653 PCA max net quantity (IATA) 11 CAO packing instructions (IATA) 660 CAO max net quantity (IATA) 30L Special provision (IATA) : A4, A137 ERG code (IATA) : 6C

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, except for:

1H,1H-Heptafluorobutyl trifluoromethanesulfonate CAS-No. 6401-01-0 100%

15.2. International regulations

CANADA

No additional information available

EU-Regulations

No additional information available

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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, developmental and/or reproductive harm

SECTION 16: Other information

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Full text of H-phrases	
H301	Toxic if swallowed
H311	Toxic in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H331	Toxic 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

NFPA reactivity

 0 - Material that in themselves are normally stable, even under fire conditions. 3 0

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