

3-Nitrobenzotrifluoride

Safety Data Sheet 4854303

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

Date of issue: 03/25/2016

Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: 3-Nitrobenzotrifluoride
CAS No	: 98-46-4
Product code	: 4854-3-03
Formula	: C7H4F3NO2
Synonyms	: 3-(Trifluoromethyl)-1-nitrobenzene
Other means of identification	: MFCD00007260

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. 4	H227 - Combustible liquid
Acute Tox. 4 (Oral)	H302 - Harmful if swallowed
Acute Tox. 4 (Dermal)	H312 - Harmful in contact with skin
Acute Tox. 1 (Inhalation)	H330 - Fatal 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
Aquatic Acute 3	H402 - Harmful to aquatic life

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US) :



GHS06

GHS07

Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H227 - Combustible liquid
H302+H312 - Harmful if swallowed or in contact with skin
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H330 - Fatal if inhaled
H335 - May cause respiratory irritation
H402 - Harmful to aquatic life

Precautionary statements (GHS-US) :

P210 - Keep away from heat/sparks/open flames/hot surfaces. No smoking
P260 - Do not breathe 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
P273 - Avoid release to the environment
P280 - Wear protective gloves/protective clothing/eye protection/face protection

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P284 - In case of inadequate ventilation wear respiratory 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
P310 - Immediately call a POISON CENTER or doctor/ physician
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
P337+P313 - If eye irritation persists: Get medical advice/attention
P362+P364 - Take off contaminated clothing and wash it before reuse
P370+P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
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

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)
3-Nitrobenzotrifluoride (Main constituent)	(CAS No) 98-46-4	<= 100	Flam. Liq. 4, H227 Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Acute Tox. 1 (Inhalation), H330 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335 Aquatic Acute 3, H402

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.

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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

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".
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

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

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.
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.
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.

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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	: Pale straw-colored, thin oily liquid.
Color	: light yellow
Odor	: aromatic
Odor threshold	: No data available
pH	: No data available
Melting point	: -1.32 °C
Freezing point	: No data available
Boiling point	: 202.75 °C
Flash point	: 88 °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	: 0.3 hPa (at 20 °C)
Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Specific gravity / density	: 1.436 g/ml (@ 25 °C)
Molecular mass	: 191.11 g/mol
Solubility	: Water: 0.4 g/l (at 20 °C)
Log Pow	: 2.6
Auto-ignition temperature	: 475 °C (at 1013 hPa)
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

9.2. Other information

Refractive index	: 1.4715 (@ 20 °C)
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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 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.

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SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed. Dermal: Harmful in contact with skin. Inhalation: Fatal if inhaled.

3-Nitrobenzotrifluoride (98-46-4)	
LD50 oral rat	610 mg/kg
LD50 dermal rat	1900 mg/kg
ATE US (oral)	610.000 mg/kg body weight
ATE US (dermal)	1900.000 mg/kg body weight
ATE US (gases)	10.000 ppmV/4h
ATE US (vapors)	0.050 mg/l/4h
ATE US (dust, mist)	0.005 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
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

3-Nitrobenzotrifluoride (98-46-4)	
LC50 fish 1	35 mg/l (Exposure time: 96 h - Species: Brachydanio rerio [static])

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

3-Nitrobenzotrifluoride (98-46-4)	
Log Pow	2.6

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 : UN2306 Nitrobenzotrifluorides, liquid, 6.1, II

UN-No.(DOT) : UN2306

Proper Shipping Name (DOT) : Nitrobenzotrifluorides, liquid

Transport hazard class(es) (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132

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Hazard labels (DOT) : 6.1 - Poison



Packing group (DOT) : II - Medium Danger

Marine pollutant : Yes (IMDG only)



DOT Packaging Non Bulk (49 CFR 173.xxx) : 202

DOT Packaging Bulk (49 CFR 173.xxx) : 243

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 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 : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.

DOT Vessel Stowage Other : 40 - Stow "clear of living quarters"

Other information : No supplementary information available.

TDG

No additional information available

Transport by sea

UN-No. (IMDG) : 2306

Proper Shipping Name (IMDG) : NITROBENZOTRIFLUORIDES, LIQUID

Class (IMDG) : 6.1 - Toxic substances

Packing group (IMDG) : II - substances presenting medium danger

Air transport

UN-No. (IATA) : 2306

Proper Shipping Name (IATA) : Nitrobenzotrifluorides, liquid

Class (IATA) : 6.1 - Toxic Substances

Packing group (IATA) : II - Medium Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

3-Nitrobenzotrifluoride (98-46-4)

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

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

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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

3-Nitrobenzotrifluoride (98-46-4)

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

EU-Regulations

No additional information available

National regulations

3-Nitrobenzotrifluoride (98-46-4)

Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)
Listed on the Canadian IDL (Ingredient Disclosure List)

15.3. US State regulations

3-Nitrobenzotrifluoride (98-46-4)

State or local regulations	U.S. - New Jersey - Right to Know Hazardous Substance 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

Full text of H-phrases:

Acute Tox. 1 (Inhalation)	Acute toxicity (inhalation) Category 1
Acute Tox. 4 (Dermal)	Acute toxicity (dermal) Category 4
Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Aquatic Acute 3	Hazardous to the aquatic environment - Acute Hazard Category 3
Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Flam. Liq. 4	Flammable liquids Category 4
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H227	Combustible liquid
H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H330	Fatal if inhaled
H335	May cause respiratory irritation
H402	Harmful to aquatic life

NFPA health hazard

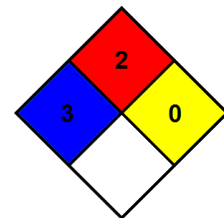
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

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

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.

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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.