

ALFAAL05948

3-Nitrobenzotrifluoride

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: Product Description:	3-硝基三氟甲苯 3-Nitrobenzotrifluoride
Cat No. :	L05948
Synonyms	3-Nitrobenzotrifluoride
CAS No	98-46-4
Molecular Formula	C7 H4 F3 N O2
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / Europe call: +32 14 57 52 11 Emergency Number US :001-201-796-7100 / Europe : +32 14 57 52 99 CHEMTREC Tel. No. US :001-800-424-9300 / Europe :001-703-527-3887
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State	Appearance	Odor
Liquid	Yellow	aromatic
Emergency Overview		
Harmful if swallowed. Harmful to aquatic life with long lasting effects. Combustible liquid. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Fatal if inhaled. May cause respiratory irritation.		

Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 1
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3
Chronic aquatic toxicity	Category 3

Label Elements

3-Nitrobenzotrifluoride

**Signal Word****Danger****Hazard Statements**

H227 - Combustible liquid
 H412 - Harmful to aquatic life with long lasting effects
 H315 - Causes skin irritation
 H319 - Causes serious eye irritation
 H330 - Fatal if inhaled
 H335 - May cause respiratory irritation
 H302 + H312 - Harmful if swallowed or in contact with skin

Precautionary Statements**Prevention**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
 P264 - Wash face, hands and any exposed 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
 P284 - Wear respiratory protection

Response

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
 P330 - Rinse mouth
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
 P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed
 P405 - Store locked up

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Combustible material.

Health Hazards

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Fatal if inhaled. May cause respiratory irritation.

Environmental hazards

Harmful to aquatic life with long lasting effects. . Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
3-Nitrobenzotrifluoride	98-46-4	97

SECTION 4. FIRST AID MEASURES

3-Nitrobenzotrifluoride

Eye Contact

Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required.

Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required.

Ingestion

Call a physician immediately. Clean mouth with water.

Most important symptoms and effects

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Combustible material. Flammable. Containers may explode when heated.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage. Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Wear self-contained breathing apparatus and protective suit. Do not let this chemical enter the environment. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE

3-Nitrobenzotrifluoride

Handling

Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Handle product only in closed system or provide appropriate exhaust ventilation. Keep away from open flames, hot surfaces and sources of ignition.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters**

Component	China	Taiwan	Thailand	Hong Kong
3-Nitrobenzotrifluoride	-	TWA: 2.5 mg/m ³	TWA: 2.5 mg/m ³	-

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
3-Nitrobenzotrifluoride	TWA: 2.5 mg/m ³	(Vacated) TWA: 2.5 mg/m ³	IDLH: 250 mg/m ³	-	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists

OSHA - Occupational Safety and Health Administration

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

Exposure Controls**Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

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Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141
When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

Environmental exposure controls Prevent product from entering drains.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Yellow	
Physical State	Liquid	
Odor	aromatic	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-5 °C / 23 °F	
Softening Point	No data available	
Boiling Point/Range	200 - 205 °C / 392 - 401 °F	@ 760 mmHg
Flash Point	87 °C / 188.6 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	Lower 1.2 Upper 18.9	
Vapor Pressure	0.3 hPa @ 20 °C	
Vapor Density	6.59	(Air = 1.0)
Specific Gravity / Density	1.430	
Bulk Density	Not applicable	Liquid
Water Solubility	0.4 g/l (20°C)	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
3-Nitrobenzotrifluoride	2.6	
Autoignition Temperature	475 °C / 887 °F	
Decomposition Temperature	> 370°C	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C7 H4 F3 N O2	
Molecular Weight	191.11	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.

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Materials to avoid Strong oxidizing agents. Strong bases. Strong reducing agents.

Hazardous Decomposition Products Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Gaseous hydrogen fluoride (HF).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
3-Nitrobenzotrifluoride	LD50 = 610 mg/kg (Rat)	LD50 = 1900 mg/kg (Rat)	

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Results / Target organs Respiratory system

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects

Do not empty into drains. Contains a substance which is: Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
3-Nitrobenzotrifluoride	LC50: = 35 mg/L, 96h			EC50 = 129.3 mg/L 16 h

3-Nitrobenzotrifluoride

	static (Brachydanio rerio)			
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Persistence and Degradability**Persistence**

Persistence is unlikely.

Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential

Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
3-Nitrobenzotrifluoride	2.6	No data available

Mobility in soil

The product is water soluble, and may spread in water systems. Will likely be mobile in the environment due to its water solubility. Highly mobile in soils.

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors.

Persistent Organic Pollutant

This product does not contain any known or suspected substance.

Ozone Depletion Potential

This product does not contain any known or suspected substance.

SECTION 13. DISPOSAL CONSIDERATIONS**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

Other Information

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not let this chemical enter the environment.

SECTION 14. TRANSPORT INFORMATION**Road and Rail Transport**

UN-No	UN2306
Proper Shipping Name	NITROBENZOTRI-FLUORIDES, LIQUID
Hazard Class	6.1
Packing Group	II

IMDG/IMO

UN-No	UN2306
Proper Shipping Name	NITROBENZOTRIFLUORIDES, LIQUID
Hazard Class	6.1
Packing Group	II

IATA

UN-No	UN2306
Proper Shipping Name	NITROBENZOTRIFLUORIDES, LIQUID
Hazard Class	6.1
Packing Group	II

Special Precautions for User

No special precautions required

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SECTION 15. REGULATORY INFORMATION

International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3-Nitrobenzotrifluoride	-	X	X	X	202-670-1	X	-	X	X	X	-	-

National Regulations

SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 27-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet