

**Safety Data Sheet**

according to UK REACH Regulation

**N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine**

Revision date: 22.03.2022

Product code: 1371

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1. Product identifier**

N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine

**Further trade names**

Carbonic acid, 4-[2-[(trifluoroacetyl)amino]ethyl]-5-(trimethylstannyl)-1,2-phenylene bis(1,1-dimethylethyl) ester

**Synonyms:**

N-trifluoroacetyl-(3,4-O-di-Boc-6-trimethylstannylphenyl)ethylamine

CAS No: 170953-68-1

**1.2. Relevant identified uses of the substance or mixture and uses advised against****Use of the substance/mixture**

Precursor for 6-[18F]Fluorodopamine

**1.3. Details of the supplier of the safety data sheet**

Company name:	ABX advanced biochemical compounds	
	Biomedizinische Forschungsreagenzien GmbH	
Street:	Heinrich-Gläser-Straße 10-14	
Place:	01454 Radeberg	
Telephone:	+49 3528 4041 60	Telefax: +49 3528 4041 65
e-mail:	info@abx.de	
Contact person:	Dr. Christoph Meyer	Telephone: +49 3528 4041 8732
e-mail:	meyer@abx.de	
Internet:	http://www.abx.de	

**1.4. Emergency telephone number:** +49 3528 4041 60**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****GB CLP Regulation**

Acute Tox. 3; H301  
 Acute Tox. 4; H312  
 Skin Irrit. 2; H315  
 Eye Irrit. 2; H319  
 STOT RE 1; H372  
 Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

**2.2. Label elements****GB CLP Regulation****Signal word:** Danger**Pictograms:****Hazard statements**

H301	Toxic if swallowed.
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.

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H372 Causes damage to organs through prolonged or repeated exposure.

H410 Very toxic to aquatic life with long lasting effects.

**Precautionary statements**

P273 Avoid release to the environment.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.

P314 Get medical advice/attention if you feel unwell.

P501 Dispose of contents/container to ....

**SECTION 3: Composition/information on ingredients****3.1. Substances****Chemical characterization**

Carbonic acid, 4-[2-[(trifluoroacetyl)amino]ethyl]-5-(trimethylstannyl)-1,2-phenylene bis(1,1-dimethylethyl) ester

Sum formula: C<sub>23</sub>H<sub>34</sub>F<sub>3</sub>NO<sub>7</sub>Sn

Molecular weight: 612.22

**Hazardous components**

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
170953-68-1	N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine			95 - < 100 %
	Acute Tox. 3, Acute Tox. 4, Skin Irrit. 2, Eye Irrit. 2, STOT RE 1, Aquatic Chronic 1; H301 H312 H315 H319 H372 H410			

Full text of H and EUH statements: see section 16.

**Specific Conc. Limits, M-factors and ATE**

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
170953-68-1		N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine	95 - < 100 %
		dermal: ATE = 1100 mg/kg; oral: ATE = 100 mg/kg	

**SECTION 4: First aid measures****4.1. Description of first aid measures****After inhalation**

Provide fresh air.

**After contact with skin**

After contact with skin, wash immediately with: Water. Change contaminated clothing.

**After contact with eyes**

Rinse immediately carefully and thoroughly with eye-bath or water.

**After ingestion**

Rinse mouth immediately and drink plenty of water. Medical treatment necessary.

**SECTION 5: Firefighting measures****5.1. Extinguishing media****Suitable extinguishing media**Water spray. Foam. Extinguishing powder. Carbon dioxide (CO<sub>2</sub>).**5.2. Special hazards arising from the substance or mixture**In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide Nitrogen oxides (NO<sub>x</sub>).

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#### **5.3. Advice for firefighters**

In case of fire: Wear self-contained breathing apparatus.

#### **Additional information**

Contaminated fire-fighting water must be collected separately. Do not allow to enter into surface water or drains.

### **SECTION 6: Accidental release measures**

#### **6.1. Personal precautions, protective equipment and emergency procedures**

##### **General advice**

Wear personal protection equipment. Provide adequate ventilation. Avoid dust formation.

#### **6.2. Environmental precautions**

Do not allow to enter into surface water or drains.

#### **6.3. Methods and material for containment and cleaning up**

##### **Other information**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal.

### **SECTION 7: Handling and storage**

#### **7.1. Precautions for safe handling**

##### **Advice on safe handling**

Do not breathe dust. If handled uncovered, arrangements with local exhaust ventilation have to be used.

##### **Advice on general occupational hygiene**

Change contaminated clothing. Wash hands before breaks and after work. When using do not eat or drink.  
Protect skin by using skin protective cream.

##### **Further information on handling**

When using do not eat, drink, smoke, sniff.

#### **7.2. Conditions for safe storage, including any incompatibilities**

##### **Requirements for storage rooms and vessels**

Keep container dry. Keep container tightly closed.

##### **Further information on storage conditions**

storage temperature:

of °C: -25

up to °C: -15

Protect against: Light.

Store under (Gas): argon. Nitrogen.

### **SECTION 8: Exposure controls/personal protection**

#### **8.1. Control parameters**

##### **Additional advice on limit values**

To date, no national critical limit values exist.

#### **8.2. Exposure controls**

##### **Individual protection measures, such as personal protective equipment**

##### **Eye/face protection**

Eye protection: Tightly sealed safety glasses.

##### **Hand protection**

Tested protective gloves are to be worn: Single-use gloves. NBR (Nitrile rubber).

##### **Skin protection**

Body protection: Lab apron. Chemical resistant safety shoes.

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**Respiratory protection**

With correct and proper use, and under normal conditions, breathing protection is not required.

**SECTION 9: Physical and chemical properties****9.1. Information on basic physical and chemical properties**

Physical state: solid  
 Colour: whitish

**Changes in the physical state****Solubility in other solvents**

Chloroform Diethyl ether

**SECTION 10: Stability and reactivity****10.4. Conditions to avoid**

Light.

**10.6. Hazardous decomposition products**

Carbon dioxide. Carbon monoxide. Nitrogen oxides (NOx). Toxic metal oxide smoke.  
 Fluorines-carbon-hydrogens.

**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in GB CLP Regulation****Acute toxicity**

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
170953-68-1	N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine				
	oral	ATE 100 mg/kg			
	dermal	ATE 1100 mg/kg			

**Carcinogenic/mutagenic/toxic effects for reproduction**

No information available.

**Practical experience**

Classification: analog Hexabutyltin; CAS 813-19-4

**SECTION 12: Ecological information****12.5. Results of PBT and vPvB assessment**

This substance does not meet the PBT/vPvB criteria of UK REACH.

**12.6. Endocrine disrupting properties**

This substance does not have endocrine disrupting properties with respect to non-target organisms.

**Further information**

Do not allow to enter into surface water or drains.

**SECTION 13: Disposal considerations****13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Dispose of waste according to applicable legislation.

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**List of Wastes Code - residues/unused products**

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

**List of Wastes Code - used product**

160508 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; discarded organic chemicals consisting of or containing hazardous substances; hazardous waste

**List of Wastes Code - contaminated packaging**

150110 WASTE PACKAGING; ABSORBENTS, WIPING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); packaging containing residues of or contaminated by hazardous substances; hazardous waste

**Contaminated packaging**

Non-contaminated packages may be recycled. Handle contaminated packages in the same way as the substance itself.

**SECTION 14: Transport information****Land transport (ADR/RID)**

**14.1. UN number or ID number:** UN 3146  
**14.2. UN proper shipping name:** ORGANOTIN COMPOUND, SOLID, N.O.S.  
 (N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine)  
**14.3. Transport hazard class(es):** 6.1  
**14.4. Packing group:** III  
 Hazard label: 6.1  
 Classification code: T3  
 Special Provisions: 43 274  
 Limited quantity: 5 kg  
 Excepted quantity: E1  
 Transport category: 2  
 Hazard No: 60  
 Tunnel restriction code: E

**Inland waterways transport (ADN)**

**14.1. UN number or ID number:** UN 3146  
**14.2. UN proper shipping name:** ORGANOTIN COMPOUND, SOLID, N.O.S.  
 (N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine)  
**14.3. Transport hazard class(es):** 6.1  
**14.4. Packing group:** III  
 Hazard label: 6.1  
 Classification code: T3  
 Special Provisions: 43 274 802  
 Limited quantity: 5 kg  
 Excepted quantity: E1

**Marine transport (IMDG)**

**14.1. UN number or ID number:** UN 3146  
**14.2. UN proper shipping name:** ORGANOTIN COMPOUND, SOLID, N.O.S.  
 (N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine)  
**14.3. Transport hazard class(es):** 6.1  
**14.4. Packing group:** III

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Hazard label:	6.1
Marine pollutant:	P
Special Provisions:	43, 223, 274
Limited quantity:	5 kg
Excepted quantity:	E1
EmS:	F-A, S-A

**Air transport (ICAO-TI/IATA-DGR)****14.1. UN number or ID number:** UN 3146**14.2. UN proper shipping name:** ORGANOTIN COMPOUND, SOLID, N.O.S.  
(N-Trifluoroacetyl-3,4-di-tert-butoxycarbonyloxy-6-trimethylstannyl-phenethylamine)**14.3. Transport hazard class(es):** 6.1**14.4. Packing group:** III

Hazard label:	6.1
Special Provisions:	A3 A5 A6
Limited quantity Passenger:	10 kg
Passenger LQ:	Y645
Excepted quantity:	E1
IATA-packing instructions - Passenger:	670
IATA-max. quantity - Passenger:	100 kg
IATA-packing instructions - Cargo:	677
IATA-max. quantity - Cargo:	200 kg

**SECTION 15: Regulatory information****15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Restrictions on use (REACH, annex XVII):  
Entry 75

**National regulatory information**

Water hazard class (D): 3 - highly hazardous to water

**SECTION 16: Other information****Relevant H and EUH statements (number and full text)**

H301	Toxic if swallowed.
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H372	Causes damage to organs through prolonged or repeated exposure.
H410	Very toxic to aquatic life with long lasting effects.