according to UK REACH Regulation

TriBoc-L-DOPA methyl ester

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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

TriBoc-L-DOPA methyl ester

Further trade names

L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-5-[[(1,1-dimethylethoxy)carbonyl]oxy]-2-(trimethylstannyl)-, methyl ester, 1,1-dimethylethyl carbonate (ester)

Synonyms:

N-tert-butoxycarbonyl-3,4-di-tert-butoxycarbonyloxy-6-(trimethylstannyl)-L-phenylalanine methyl ester

CAS No: 857502-21-7

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

Use of the substance/mixture

Stannylated precursor for 6-[18F]Fluoro-L-DOPA

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

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 +49 3528 4041 60

number:

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

Hazard components for labelling

TriBoc-L-DOPA methyl ester **Signal word:**Danger

Pictograms:







Hazard statements

H301 Toxic if swallowed.

according to UK REACH Regulation

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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.		
Precautionary statemen	nts		
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.		

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-5-[[(1,1-dimethylethoxy)carbonyl]oxy]-2-(trimethylstannyl)-, methyl

ester, 1,1-dimethylethyl carbonate (ester)

Sum formula: C28H45NO10Sn

Molecular weight: 647.37

Hazardous components

CAS No	Chemical name				Quantity
	EC No	Index No	REACH N	lo	
	Classification (GB CLP Regulation)				
857502-21-7	TriBoc-L-DOPA methyl ester		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

opeonic contraction and the			
CAS No	EC No	Chemical name	Quantity
	Specific Conc. L	Limits, M-factors and ATE	
857502-21-7		TriBoc-L-DOPA methyl ester	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 (CO2).

according to UK REACH Regulation

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5.2. Special hazards arising from the substance or mixture

In case of fire may be liberated: Carbon dioxide (CO2). Carbon monoxide Nitrogen oxides (NOx).

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).

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Skin protection

Body protection: Lab apron. Chemical resistant safety shoes.

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: colourless

Changes in the physical state

Melting point/freezing point:

44 - 49 °C

Water solubility:

practically insoluble

Solubility in other solvents

Chloroform

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.

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
857502-21-7	TriBoc-L-DOPA methyl ester				
	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

according to UK REACH Regulation

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13.1. Waste treatment methods

Disposal recommendations

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

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. (Trimethyltin-dopa-derivate)

14.3. Transport hazard class(es): 6.1 14.4. Packing group: Ш Hazard label: 6.1 Classification code: T3 **Special Provisions:** 43 274 Limited quantity: 5 kg Excepted quantity: F1 Transport category: 2 Hazard No: 60 Tunnel restriction code: F

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. (Trimethyltin-dopa-derivate)

14.3. Transport hazard class(es):6.114.4. Packing group:IIIHazard label:6.1Classification 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. (Trimethyltin-dopa-derivate)

14.3. Transport hazard class(es):6.114.4. Packing group:IIIHazard label:6.1Marine pollutant:P

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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. (Trimethyltin-dopa-derivate)

14.3. Transport hazard class(es):6.114.4. Packing group:IIIHazard label:6.1Special Provisions:A3 A5 A6Limited quantity Passenger:10 kgPassenger LQ:Y645Excepted 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.