

Safety Data Sheet

according to UK REACH Regulation

isoSGMIB precursor

Revision date: 16.06.2022

Product code: 7021

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

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Further trade names

Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl] [[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]methyl]-5-(trimethylstannyl)-2,5-dioxo-1-pyrrolidinyl ester

synonyms: N-Succinimidyl-3-(1,2-bis-BOC-guanidino)-methyl-5-(trimethylstannyl)-benzoate.

1.2. Relevant identified uses of the substance or mixture and uses advised against**Use of the substance/mixture**isoSGMIB precursor may be used as precursor for [¹³¹I]isoSGMIB.**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****Hazard components for labelling**

Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl] [[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]methyl]-5-(trimethylstannyl)-2,5-dioxo-1-pyrrolidinyl ester

Signal word: Danger**Pictograms:****Hazard statements**

H301 Toxic if swallowed.

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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 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.
P302+P352	IF ON SKIN: Wash with plenty of water.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314	Get medical advice/attention if you feel unwell.

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

Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl]][(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]methyl]-5-(trimethylstannyl)-2,5-dioxo-1-pyrrolidinyl ester

Sum formula: C₂₆H₃₈N₄O₈Sn

Molecular weight: 653,31

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
	Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl]][(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]methyl]			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	
		Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl]][(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]amino]methyl]	95 - < 100 %
		dermal: ATE = 1100 mg/kg; oral: ATE = 100 mg/kg	

SECTION 4: First aid measures**4.1. Description of first aid measures****General information**

First aider: Pay attention to self-protection!

After inhalation

No mouth-to-mouth or mouth-to-nose resuscitation. Use Ambu bag or ventilator. Call a physician immediately. Provide fresh air. In case of breathing difficulties administer oxygen. In all cases of doubt, or when symptoms persist, seek medical advice.

After contact with skin

Medical treatment necessary. After contact with skin, wash immediately with: Water. Change contaminated clothing. Seek medical advice.

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After contact with eyes

In case of contact with eyes, rinse immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart. Subsequently consult an ophthalmologist.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**

Suitable extinguishing media: Water spray. Foam. Extinguishing powder. Carbon dioxide (CO₂).

5.2. Special hazards arising from the substance or mixture

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

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

Additional information

Suppress gases/vapours/mists with water spray jet. 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**

Provide adequate ventilation. Avoid dust formation. Do not breathe dust. Avoid contact with skin, eyes and clothes. Wear personal protection equipment.

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. Avoid dust formation. Clear contaminated areas thoroughly.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

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

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Protect skin by using skin protective cream. After work, wash hands and face. Do not eat, drink, smoke or sneeze at the workplace.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container dry. Keep locked up. Store in a place accessible by authorized persons only. Keep container tightly closed in a cool, well-ventilated place. Restrict access to stockrooms.

Further information on storage conditions

storage temperature:

of °C:-25

up to °C:-15

Store under (Gas): argon. Nitrogen.

Protect against: Light.

SECTION 8: Exposure controls/personal protection

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8.1. Control parameters**Additional advice on limit values**

To date, no national critical limit values exist.

8.2. Exposure controls**Appropriate engineering controls**

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

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

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

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

Water solubility: The study does not need to be conducted
 because the substance is known to be
 insoluble in water.

Solubility in other solvents

Chloroform, Dimethylformamide Methanol. ethyl acetate.

SECTION 10: Stability and reactivity**10.5. Incompatible materials**

Water. Oxidizing agents, strong.

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**

Toxic. Acute toxicity, oral. Acute toxicity, inhalant. Acute toxicity, dermal.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
	Benzoic acid-3-[[[(1,1-dimethylethoxy)carbonyl]][(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]ami				
	oral	ATE 100 mg/kg			
	dermal	ATE 1100 mg/kg			

Irritation and corrosivity

Irritating to eyes. After skin contact: irritant.

Carcinogenic/mutagenic/toxic effects for reproduction

Toxicological data are not available.

STOT-repeated exposure

Danger of serious damage to health by prolonged exposure.

Further information

Data obtained by analogy conclusion, e.g. QSAR.

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SECTION 12: Ecological information**12.1. Toxicity**

Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

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 uncontrolled discharge of product into the environment.

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.

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

Contaminated packaging

Non-contaminated packages may be recycled.

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 (contains Trimethyltin-dopa-derivate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

III

Hazard label:

6.1

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 (contains Trimethyltin-derivate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

III

Hazard label:

6.1

Marine transport (IMDG)**14.1. UN number or ID number:**

UN 3146

14.2. UN proper shipping name:

ORGANOTIN COMPOUND, SOLID, N.O.S (contains Trimethyltin-derivate)

14.3. Transport hazard class(es):

6.1

14.4. Packing group:

III

Hazard label:

6.1

Air transport (ICAO-TI/IATA-DGR)

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14.1. UN number or ID number:	UN 3146
14.2. UN proper shipping name:	ORGANOTIN COMPOUND, SOLID, N.O.S (contains Trimethyltin-derivate)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	III
Hazard label:	6.1

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