

Safety Data Sheet

according to UK REACH Regulation

Dimethyl-8-phenylsulfonyl-5-phenylsulfonyloxy-hexahydropyrrolo[2,3]indol-1,2-dicarboxylate

Revision date: 01.06.2022

Product code: 6520

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

1.1. Product identifier

Dimethyl-8-phenylsulfonyl-5-phenylsulfonyloxy-hexahydropyrrolo[2,3]indol-1,2-dicarboxylate

Further trade names

Pyrrolo[2,3-b]indole-1,2(2H)-dicarboxylic acid, 3,3a,8,8a-tetrahydro-8-(phenylsulfonyl)-5-[(phenylsulfonyl)oxy]-, dimethyl ester, [2S-(2alpha,3a beta,8a beta)]-

Synonyms:

Dimethyl-(2S, 3aR, 8aS)

-8-phenylsulfonyl-5-phenylsulfonyloxy-1,2,3,3a,8a-hexahydropyrrolo[2,3]indol-1,2-dicarboxylate

CAS No: 150804-39-0

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

Use of the substance/mixture

Precursor for 5-OH-a-[11C]Methyl-L-tryptophan

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

This substance is not classified as hazardous in accordance with GB CLP Regulation.

2.2. Label elements

GB CLP Regulation

Precautionary statements

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

2.3. Other hazards

Warning - substance not yet tested completely.

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

Pyrrolo[2,3-b]indole-1,2(2H)-dicarboxylic acid, 3,3a,8,8a-tetrahydro-8-(phenylsulfonyl)-5-[(phenylsulfonyl)oxy]-, dimethyl ester, [2S-(2alpha,3a beta,8a beta)]-

Sum formula: C₂₆H₂₄N₂O₉S₂

Molecular weight: 572.61

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Hazardous components

none (according to UK REACH Regulation)

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

If swallowed, immediately drink: Water. Call a physician immediately.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings. Suitable extinguishing media: Foam. Extinguishing powder. Carbon dioxide (CO₂). Atomized water.

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

6.2. 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. Conditions to avoid: skin contact. Eye contact. Wear personal protection equipment. When using do not eat, drink, smoke, sniff.

Advice on general occupational hygiene

Change contaminated clothing. Wash hands before breaks and after work. When using do not eat or drink.

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

Recommended storage temperature:

of °C: 2

up to °C: 8

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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

Appropriate engineering controls

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: white

Changes in the physical state

Melting point/freezing point: 80 - 95 °C

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. Dichloromethane: ethyl acetate.

SECTION 10: Stability and reactivity

10.4. Conditions to avoid

Light.

10.6. Hazardous decomposition products

Carbon dioxide. Carbon monoxide. Nitrogen oxides (NO_x). Sulphur dioxide.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in GB CLP Regulation

Information on likely routes of exposure

Toxicological data are not available.

Further information

Toxicological data are not available.

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

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Disposal recommendations

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

Contaminated packaging

Non-contaminated packages may be recycled.

SECTION 14: Transport information**Other applicable information**

Not a hazardous material with respect to these transportation regulations.

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