

Safety Data Sheet

according to UK REACH Regulation

Desmethyl-SCH-442416

Revision date: 10.05.2022

Product code: 3700

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

Desmethyl-SCH-442416

Further trade names

Phenol, 4-[3-[5-amino-2-(2-furanyl)-7H-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-7-yl]propyl]-

Synonyms:

5-Amino-7-[3-(4-hydroxyphenyl)propyl]-2-(2-furyl)pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine

CAS No: 188112-92-7

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

Precursor for [11C]SCH 442416

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. 5; H313

Acute Tox. 5; H303

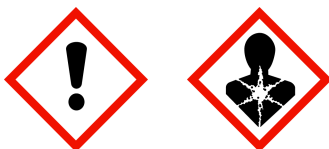
STOT SE 3; H335

STOT RE 2; H373

Full text of hazard statements: see SECTION 16.

2.2. Label elements**GB CLP Regulation****Hazard components for labelling**

Desmethyl-SCH-442416

Signal word: Warning**Pictograms:****Hazard statements**

H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H332	Harmful if inhaled.
H315+H320	Causes skin and eye irritation.

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H335 May cause respiratory irritation.

H373 May cause damage to organs through prolonged or repeated exposure.

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**

Phenol, 4-[3-[5-amino-2-(2-furanyl)-7H-pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-7-yl]propyl]-

Sum formula: C₁₉H₁₇N₇O₂

Molecular weight: 375.38

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
188112-92-7	Desmethyl-SCH-442416			95 - < 100 %
	Acute Tox. 5, Acute Tox. 5, STOT SE 3, STOT RE 2; H313 H303 H335 H373			

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	
188112-92-7		Desmethyl-SCH-442416	95 - < 100 %
		dermal: ATE = 2500 mg/kg; oral: ATE = 2500 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

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.

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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

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:

light yellow , 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

dimethylsulphoxide (DMSO).

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

Light.

10.6. Hazardous decomposition productsCarbon dioxide. Carbon monoxide. Nitrogen oxides (NO_x).**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
188112-92-7	Desmethyl-SCH-442416				
	oral	ATE 2500 mg/kg			
	dermal	ATE 2500 mg/kg			

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****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

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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**Relevant H and EUH statements (number and full text)**

H302	Harmful if swallowed.
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