

**Safety Data Sheet**

according to UK REACH Regulation

**(S)-N-Desmethyl PK11195**

Revision date: 23.03.2022

Product code: 1620

Page 1 of 4

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

(S)-N-Desmethyl PK11195

**Further trade names**

3-Isoquinolinecarboxamide, 1-(2-chlorophenyl)-N-(1-methylpropyl)-(S)

Synonyms:

1-(2-Chlorophenyl)-N-(1-methylpropyl)-isoquinoline-3-carboxamide-(S)

CAS No: 157809-86-4

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

Precursor for (S)-[N-Methyl-11C-]PK11195

**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**

3-Isoquinolinecarboxamide, 1-(2-chlorophenyl)-N-(1-methylpropyl)-(S)

Sum formula: C<sub>20</sub>H<sub>19</sub>ClN<sub>2</sub>O

Molecular weight: 338.83

**Hazardous components**

none (according to UK REACH Regulation)

**Safety Data Sheet**

according to UK REACH Regulation

**(S)-N-Desmethyl PK11195**

Revision date: 23.03.2022

Product code: 1620

Page 2 of 4

**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 (CO<sub>2</sub>). 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: -25

up to °C: -15

Protect against: Light.

Store under (Gas): argon.

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

**Safety Data Sheet**

according to UK REACH Regulation

**(S)-N-Desmethyl PK11195**

Revision date: 23.03.2022

Product code: 1620

Page 3 of 4

**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: colourless , whitish

**Changes in the physical state**

Melting point/freezing point: 127 - 130 °C

**Solubility in other solvents**

Chloroform , dimethylsulphoxide (DMSO).

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

Light.

**10.6. Hazardous decomposition products**Carbon dioxide. Carbon monoxide. Nitrogen oxides (NO<sub>x</sub>). Hydrochloric gas.**SECTION 11: Toxicological information****11.1. Information on hazard classes as defined in GB CLP Regulation****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**

**Safety Data Sheet**

according to UK REACH Regulation

**(S)-N-Desmethyl PK11195**

Revision date: 23.03.2022

Product code: 1620

Page 4 of 4

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.

**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**