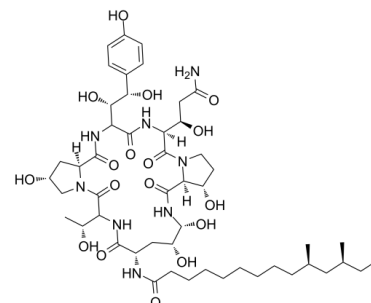


Data Sheet

Product Name:	Pneumocandin B0
Cat. No.:	CS-3247
CAS No.:	135575-42-7
Molecular Formula:	C ₅₀ H ₈₀ N ₈ O ₁₇
Molecular Weight:	1065.21
Target:	Fungal
Pathway:	Anti-infection
Solubility:	10 mM in DMSO



BIOLOGICAL ACTIVITY:

Pneumocandin B0(L-688786), a key intermediate in the synthesis of the antifungal agent, Cancidas, has led to the identification of several materials with potential for improved performance.

References:

- [1]. Welch CJ, et al. Preparation and evaluation of novel stationary phases for improved chromatographic purification of pneumocandin B0. J Chromatogr A. 2006 Jan 6;1101(1-2):204-13.
- [2]. Leonard WR Jr, et al. Synthesis of the antifungal beta-1,3-glucan synthase inhibitor CANCIDAS (caspofungin acetate) from pneumocandin B0. J Org Chem. 2007 Mar 30;72(7):2335-43.

CAIndexNames:

L-Proline, (4R,5R)-N2-[(10R,12S)-10,12-dimethyl-1-oxotetradecyl]-4,5-dihydroxy-L-ornithyl-L-threonyl-(4R)-4-hydroxy-L-prolyl-(4S)-4-hydroxy-4-(4-hydroxyphenyl)-L-threonyl-(3R)-3-hydroxy-L-glutaminy-3-hydroxy-, (6→1)-lactam, (3S)-

SMILES:

O=C([C@](NC(C(NC([C@@](C[C@@H](O)C1([H])N1C2=O)=O)[C@H](O)[C@H](C3=CC=C(O)C=C3)O)=O)([H])[C@H](O)CC(N)=O)N4[C@@](C(N[C@@H]([C@@H](C[C@@H](C(NC2[C@H](O)C)=O)NC(CCCCCC[C@@H](C)C[C@@H](C)CC=O)O)O)=O)([H])[C@@H](O)CC4

Caution: Product has not been fully validated for medical applications. For research use only.

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