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Typical Product Specifications & Properties

Flagecidin

CAS Number: : 22862-76-6

Specifications	Limits
Molecular weight	265.31
SMILES	<chem>[C@H]1([C@@H]([C@H](CN1)O)OC(=O)C)Cc1ccc(cc1)OC</chem>
InChI	YKJYKKNCCRKFSL-RDBSUJKOSA-N
InChIKey	1S/C14H19NO4/c1-9(16)19-14-12(15-8-13(14)17)7-10-3-5-11(18-2)6-4-10/h3-6,12-15,17H,7-8H2,1-2H3/t12-,13+,14+/m1/s1
log P (octanol-water)	0.610
Atmospheric OH Rate Constant	1.25E-10 cm ³ /molecule-sec
Melting Point	140.5 ° C
Water solubility	6550 mg/L



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