

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 |