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Typical Product Specifications & Properties

(25?)-16,28-Seco-5?-Solanid- 22(28)-En-3?-Ol

CAS Number: : 984-82-7

Specifications	Limits
Molecular weight	399.66
SMILES	<chem>C[C@@H]1CCC(=NC1)[C@@H](C)[C@H]2CC[C@@H]3[C@@]2(CC[C@H]4[C@H]3CC[C@@H]5[C@@](C5)O)C)C</chem>
InChI	MSKAAWFUKWQOQS-YNAJWQGRSA-N
InChIKey	1S/C27H45NO/c1-17-5-10-25(28-16-17)18(2)22-8-9-23-21-7-6-19-26(19,3)24(21)12-14-27(22,23)4/h17-24,29H,5-16H2,1-4H3/t17-,18+,19+,20+,21+,22-,23+,24+,26+,27-/m1/s1



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