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Typical Product Specifications & Properties

Neoandrographolide

CAS Number: : 27215-14-1

Specifications	Limits
Molecular weight	480.59
SMILES	<chem>C[C@@]1(CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)CCC[C@@]3(C)[C@H](CCC4=CCOC4=O)C(=C)CC[C@H]13</chem>
InChI	YGCYRQKJYWQXHG-RDNQFMDVSA-N
InChIKey	1S/C26H40O8/c1-15-5-8-19-25(2,14-33-24-22(30)21(29)20(28)18(13-27)34-24)10-4-11-26(19,3)17(15)7-6-16-9-12-32-23(16)31/h9,17-22,24,27-30H,1,4-8,10-14H2,2-3H3/t17-,18-,19-,20-,21+,22-,24-,25+,26+/m1/s1



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