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Typical Product Specifications & Properties

Stenophylline A

CAS Number: : 91450-13-4

Specifications	Limits
SMILES	<chem>C1[C@@]([C@@]2([C@@H]3C[C@H]([C@H]4[C@@H]5[C@]([C@@H]([C@@H]6[C@@H](C)[C@@H]7CC[C@H](C)C[N@@]7C[C@@H]6[C@@H]5C[C@@]4([C@@]3(C1)C)O2)C(O)C\C=C(/C(=O)O)C)O)O)(O)C\C=C(/C(=O)O)C</chem>
InChI	NQQDXUQABFCHGS-HQ SXMINWSA-N
InChIKey	1S/C37H55NO10/c1-18-6-7-24-21(4)27-23(17-38(24)16-18)22-1536-29(28(22)35(46,30(27)40)11-9-20(3)32(43)44)25(39)14-26-33(36,5)12-13-34(45,37(26,47)48-36)10-8-19(2)31(41)42/h8-9,18,21-30,39-40,45-47H,6-7,10-17H2,1-5H3,(H,41,42)(H,43,44)/b19-8-,20-9-/t1



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