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Typical Product Specifications & Properties

Crassicauline A

CAS Number: : 79592-91-9

Specifications	Limits
Molecular weight	643.77
SMILES	<chem>C1C[C@@]2(COC)C[N@@]([C@@H]3[C@@H]4[C@@H]([C@@H]2[C@@]3([C@@H]1OC)[C@@H]1C[C@@]2([C@@H](OC)C[C@@]4(OC(C)=O)[C@@H]1[C@@H]2OC(c1ccc(cc1)OC)=O)O)OC)CC</chem>
InChI	GAZDXIGXYVWQX-UHFFFAOYSA-N
InChIKey	1S/C35H49NO10/c1-8-36-17-32(18-40-3)14-13-23(42-5)35-22-15-33(39)24(43-6)16-34(46-19(2)37,26(29(35)36)27(44-7)28(32)35)25(22)30(33)45-31(38)20-9-11-21(41-4)12-10-20/h9-12,22-30,39H,8,13-18H2,1-7H3



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