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Typical Product Specifications & Properties

Isoacteoside

CAS Number: : 61303-13-7

Specifications	Limits
Molecular weight	624.59
SMILES	<chem>C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@H]2[C@@H]([C@@H]2O)OCCc3ccc(c(c3)O)O)COC(=O)/C=C/c4ccc(c(c</chem>
InChI	FNMHEHXNBNCPCI-QEOJJFGVSA-N
InChIKey	1S/C29H36O15/c1-13-22(35)24(37)25(38)29(42-13)44-27-23(36)21(34)7-4-14-2-5-16(30)18(32)10-14)43-28(26(27)39)40-9-8-15-3-17(31)19(33)11-15/h2-7,10-11,13,20,22-33,35-39H,8-9,12H2,1H3,4+/t13-,20+,22-,23+,24+,25+,26+,27-,28+,29-/m0/s1
Chemical Structure	 29601 2-(2-Chloroethoxy)ethanol chemical structure



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