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Typical Product Specifications & Properties

Chaetiacandin

CAS Number: : 96989-32-1

Specifications	Limits
Molecular weight	832.93
SMILES	<chem>O1[C@@H](c2c(cc(cc2O)O)CO)[C@@H]([C@@H]([C@@H](O[C@@H]2[C@@H](O)[C@@H]([C@@H](O2)[C@@H](O)COC(\C=C\C=C\C(CCCC)=O)O)[C@@H]1CO)OC(\C=C\C=C\C[C@@H](\C=C\C=C\C(C)C)O)=O)O</chem>
InChI	XTPPYHVGAMJHPL-WAXQHDLUSA-N
InChIKey	1S/C43H60O16/c1-4-5-6-7-8-9-12-19-33(50)55-25-31(49)39-36(52)37(53)43(58-39)59-40-32(24-45)56-41(35-27(23-44)21-29(47)22-30(35)48)38(54)42(40)57-34(51)20-13-10-11-17-28(46)18-15-14-16-26(2)3/h8-16,18-22,26,28,31-32,36-49,52-54H,4-7,17,23-25H2,1-3H3/b



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