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Typical Product Specifications & Properties

N-Benzyladriamycin-14-Valerate

CAS Number: : 98983-21-2

Specifications	Limits
Molecular weight	717.76
SMILES	<chem>c1ccc2C(c3c(c(c4c(C[C@](C(=O)COC(CCCC)=O)(O)C[C@@H]4O[C@@H]4O[C@H]([C@H]([C@H](C4)NCc4ccccc4)O)C)c3O)O)C(c2c1OC)=O)=O</chem>
InChI	IUKSGXMOHXEUJY-YWVRLZ QXSA-N
InChIKey	1S/C39H43NO12/c1-4-5-14-28(42)50-19-27(41)39(48)16-23-31(38(47)33-32(36(23)45)35(44)22-12-9-13-25(49-3)30(22)37(33)46)26(17-39)52-29-15-24(34(43)20(2)51-29)40-18-21-10-7-6-8-11-21/h6-13,20,24,26,29,34,40,43,45,47-48H,4-5,14-19H2,1-3H3/t20-,24-,26-,29



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