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Typical Product Specifications & Properties

11 β ,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-hexanoate

CAS Number: : 69164-69-8

Specifications	Limits
Molecular weight	458.59
EINECS	273-898-7
SMILES	<chem>C1(C=C[C@@]2([C@H]3[C@H](C[C@@]4([C@](CC[C@@H]4[C@@H]3CCCC2=C1)(C(COC(CCCCC)=O)=O)O)C)O)C)=O</chem>
InChI	DNSAKUGJOSFARZ-FOMYWIRZSA-N
InChIKey	1S/C27H38O6/c1-4-5-6-7-23(31)33-16-22(30)27(32)13-11-20-19-9-8-17-14-18(28)10-12-25(17,2)24(19)21(29)15-26(20,27)3/h10,12,14,19-21,24,29,32H,4-9,11,13,15-16H2,1-3H3/t19-,20-,21-,24+,25-,26-,27-/m0/s1



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