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Typical Product Specifications & Properties

2,16a,20,25-tetrahydroxy-9 β -methyl-10a-19-norlanosta-1,5,23(E)-triene-3,11,22-trione

CAS Number: : 2222-07-3

Specifications	Limits
Molecular weight	514.65
EINECS	218-736-8
SMILES	<chem>C12=CC[C@H]3[C@@]4(C[C@@H](O)[C@@H]([C@@]4(CC([C@@]3([C@@H]2C=C(O)C(C1(C)C)=O)C)=O)C[C@](C(\C=C\C(O)(C)C)=O)(O)C)C</chem>
InChI	NISPVUDLMHQFRQ-MKIKIEMVSA-N
InChIKey	1S/C30H42O7/c1-25(2,36)12-11-21(33)30(8,37)23-19(32)14-27(5)20-10-9-16-17(13-18(31)24(35)26(16,3)4)29(20,7)22(34)15-28(23,27)6/h9,11-13,17,19-20,23,31-32,36-37H,10,14-15H2,1-8H3/b12-11+/t17-,19-,20+,23+,27+,28-,29+,30+/m1/s1



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