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Typical Product Specifications & Properties

11 β ,17,21-trihydroypregn-4-ene-3,20-dione 21-(dihydrogen phosphate)

CAS Number: : 3863-59-0

Specifications	Limits
Molecular weight	442.44
EINECS	223-382-2
SMILES	<chem>C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)COP(=O)(O)O)[C@@]4(C)C[C@H](O)[C@H]23</chem>
InChI	BGSOJVFOEQIVMH-VWUMJDOOSA-N
InChIKey	1S/C21H31O8P/c1-19-7-5-13(22)9-12(19)3-4-14-15-6-8-21(25,17(24)11-29-30(26,27)28)20(15,2)10-16(23)18(14)19/h9,14-16,18,23,25H,3-8,10-11H2,1-2H3,(H2,26,27,28)/t14-,15-,16-,18+,19-,20-,21-/m0/s1



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