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Typical Product Specifications & Properties

11 β ,17,21-trihydroxypregn-4-ene-3,20-dione 17-benzoate

CAS Number: : 28956-89-0

Specifications	Limits
Molecular weight	466.57
EINECS	249-328-8
SMILES	<chem>C=12[C@@]([C@H]3[C@H](C[C@@]4[C@@](OC(=O)c5ccccc5)(C(=O)CO)CC[C@@H]4[C@@H]3CC2)C)O)(CCC(=O)C1)C</chem>
InChI	LPEYMYDYPGRLBU-YGZHYJPASA-N
InChIKey	1S/C28H34O6/c1-26-12-10-19(30)14-18(26)8-9-20-21-11-13-28(23(32)16-29,27(21,2)15-22(31)24(20)26)34-25(33)17-6-4-3-5-7-17/h3-7,14,20-22,24,29,31H,8-13,15-16H2,1-2H3/t20-,21-,22-,24+,26-,27-,28-/m0/s1



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