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## Typical Product Specifications & Properties

# 11 $\beta$ ,17,21-trihydroxypregna-1,4-diene-3,20-dione 17-benzoate

CAS Number: : 31311-74-7

Specifications	Limits
Molecular weight	464.55
EINECS	250-562-8
SMILES	<chem>[C@]12([C@@](OC(=O)c3ccccc3)(C(=O)CO)CC[C@H]1[C@H]1[C@@H]([C@@]3(C(=CC(=O)C=C3)CC1)C)[C@H](C2)O)C</chem>
InChI	SUJDKANSELPHHZ-YGZHYJPASA-N
InChIKey	1S/C28H32O6/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/h3-7,10,12,14,20-22,24,29,31H,8-9,11,13,15-16H2,1-2H3/t20-,21-,22-,24+,26-,27-,28-/m0/s1



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