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## Typical Product Specifications & Properties

# 11 $\beta$ ,17,21-trihydroxypregn-4-ene-3,20-dione 21-hexanoate

CAS Number: : 3593-96-2

Specifications	Limits
Vapor Pressure	4.54E-15 mm Hg
log P (octanol-water)	4.48
Water solubility	0.191 mg/L
Atmospheric OH Rate Constant	1.17E-10 cm <sup>3</sup> /molecule-sec
Henry's Law Constant	1.94E-11 atm-m <sup>3</sup> /mole
Molecular weight	460.60
EINECS	222-737-9
SMILES	<chem>C=12[C@@](CCC(C1)=O)(C)[C@H]1[C@H](C[C@@]3([C@H]([C@@H]1CC2)CC[C@@]3(C(COC(=O)CCCC)=O)O)C)O</chem>
InChI	XZSVYVIYKBHVMV-FOMYWIRZSA-N
InChIKey	1S/C27H40O6/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/h14,19-21,24,29,32H,4-13,15-16H2,1-3H3/t19-,20-,21-,24+,25-,26-,27-/m0/s1



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