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Typical Product Specifications & Properties

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

CAS Number: : 6677-99-2

Specifications	Limits
Molecular weight	432.55
EINECS	229-715-8
SMILES	<chem>CCCC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C</chem>
InChI	YZNQMPPBWQTLFJ-TUFAYURCSA-N
InChIKey	1S/C25H36O6/c1-4-5-21(29)31-14-20(28)25(30)11-9-18-17-7-6-15-12-16(26)8-10-23(15,2)22(17)19(27)13-24(18,25)3/h12,17-19,22,27,30H,4-11,13-14H2,1-3H3/t17-,18-,19-,22+,23-,24-,25-/m0/s1
Atmospheric OH Rate Constant	1.15E-10 cm ³ /molecule-sec
Vapor Pressure	3.43E-14 mm Hg
Henry's Law Constant	1.10E-11 atm-m ³ /mole
log P (octanol-water)	2.91
Water solubility	3.690 mg/L

