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Typical Product Specifications & Properties

11 β ,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-octanoate

CAS Number: : 85959-58-6

Specifications	Limits
Molecular weight	486.64
EINECS	289-053-0
SMILES	<chem>CCCCCCCC(=O)OCC(=O)[C@]1(CC[C@@H]2[C@@]1(C[C@@H]([C@H]3[C@H]2CCC4=CC(=O)C=C[C@]34C)O)C)O</chem>
InChI	NDWSWWNCJPFKAB-KAQKJVHQSA-N
InChIKey	1S/C29H42O6/c1-4-5-6-7-8-9-25(33)35-18-24(32)29(34)15-13-22-21-11-10-19-16-20(30)12-14-27(19,2)26(21)23(31)17-28(22,29)3/h12,14,16,21-23,26,31,34H,4-11,13,15,17-18H2,1-3H3/t21-,22-,23-,26+,27-,28-,29-/m0/s1



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