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Typical Product Specifications & Properties

11 β ,17,21-trihydroxy-6 α -methylpregna-1,4-diene-3,20-dione 21-acetylsalicylate

CAS Number: : 94135-36-1

Specifications	Limits
Molecular weight	536.61
EINECS	302-905-9
SMILES	<chem>[C@@]12(C=CC(=O)C=C2)[C@H](C[C@@H]2[C@@H]1[C@H](C[C@@]1([C@@](C(=O)COC(=O)c3c(OC(=O)C)cccc3)(CC[C@H]21)O)C)O)C</chem>
InChI	YOFQBOKKLYIOGE-NOQXCBQUSA-N
InChIKey	1S/C31H36O8/c1-17-13-21-22-10-12-31(37,26(35)16-38-28(36)20-7-5-6-8-25(20)39-18(2)32)30(22,4)15-24(34)27(21)29(3)11-9-19(33)14-23(17)29/h5-9,11,14,17,21-22,24,27,34,37H,10,12-13,15-16H2,1-4H3/t17-,21-,22-,24-,27+,29-,30-,31-/m0/s1



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