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Typical Product Specifications & Properties

11 β ,17-dihydroxypregna-1,4-diene-3,20-dione 21-[(6-carboxycyclohex-3-en-1-yl)formate]

CAS Number: : 3331-71-3

Specifications	Limits
Molecular weight	512.59
EINECS	222-058-8
SMILES	<chem>C=12[C@@](C=CC(C1)=O)(C)[C@H]1[C@H](C[C@@]3([C@H]([C@@H]1CC2)CC[C@@]3(C(COC([C@@H]1[C@@H](C(=O)O)CC=CC1)=O)=O)O)C)O</chem>
InChI	VNGWBSXDGQZ SFL-JMNKGBLSA-N
InChIKey	1S/C29H36O8/c1-27-11-9-17(30)13-16(27)7-8-20-21-10-12-29(36,28(21,2)14-22(31)24(20)27)23(32)15-37-26(35)19-6-4-3-5-18(19)25(33)34/h3-4,9,11,13,18-22,24,31,36H,5-8,10,12,14-15H2,1-2H3,(H,33,34)/t18?,19?,20-,21-,22-,24+,27-,28-,29-/m0/s1



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