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Typical Product Specifications & Properties

11a,17,21-trihydroxy-16a-methylpregna-1,4-diene-3,20-dione

CAS Number: : 78761-59-8

Specifications	Limits
Molecular weight	374.47
EINECS	278-982-7
SMILES	<chem>C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@@]4([C@H](C[C@@]2([C@]1(C(=O)CO)O)C)O)C</chem>
InChI	WNYLPFCKNQAAMB-JPDWDDBRSA-N
InChIKey	1S/C22H30O5/c1-12-8-16-15-5-4-13-9-14(24)6-7-20(13,2)19(15)121(16,3)22(12,27)18(26)11-23/h6-7,9,12,15-17,19,23,25,27H,4-5,11H2,1-3H3/t12-,15+,16+,17-,19-,20+,21+,22+/m1/s1



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