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Typical Product Specifications & Properties

17 α -hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one

CAS Number: : 2787-02-2

Specifications	Limits
Molecular weight	340.46
EINECS	220-513-5
SMILES	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@]2(C#C)O)CCC4=CC(=O)/C(=C\O)/C[C@]3</chem>
InChI	FYEOMZSZJFOTGQ-GXWGVVPSA-N
InChIKey	1S/C22H28O3/c1-4-22(25)10-8-18-16-6-5-15-11-19(24)14(13-23)20(15,2)17(16)7-9-21(18,22)3/h1,11,13,16-18,23,25H,5-10,12H2,3H3/b14-13-/t16-,17+,18+,20+,21+,22+/m1/s1



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