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Typical Product Specifications & Properties

Pregnane-3,20-Dione, (5.Beta.)-

CAS Number: : 128-23-4

Specifications	Limits
Molecular weight	316.48
SMILES	<chem>O=C1C[C@H]2CC[C@H]3[C@@H]4CC[C@@H]([C@@]4(CC[C@H]3[C@@]2(CC1)C)C)C(=O)C</chem>
InChI	1S/C21H32O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-21(17,18)3/h14,16-19H,4-12H2,1-3H3/t14-,16+,17-,18+,19+,20+,21-/m0/s1
InChIKey	XMRPGKVKISIQBV-IWQCLKLKSA-N
log P (octanol-water)	3.460
Melting Point	123 ° C
Atmospheric OH Rate Constant	3.85E-11 cm ³ /molecule-sec



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415 Huguenot Street, New Rochelle, New York 10801

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