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Typical Product Specifications & Properties

11-Deoxycorticosterone

CAS Number: : 64-85-7

Specifications	Limits
Molecular weight	330.46
EINECS	200-596-4
InChI	1S/C21H30O3/c1-20-9-7-14(23)11-13(20)3-4-15-16-5-6-18(19(24)12-22)21(16,2)10-8-17(15)20/h11,15-18,22H,3-10,12H2,1-2H3/t15-,16-,17-,18+,20-,21-/m1/s1
InChIKey	ZESRJSPZRDMNHY-VQBCACJISA-N
Alpha	184 ° (c=1, C ₂ H ₅ OH)
Melting Point	138-144 °C
Storage Temperature	?20°C
Water solubility	slightly soluble
Merck	13,2917
Flash Point	9?
Molecular weight	372.50
EINECS	200-275-9





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Specifications	Limits
SMILES	<chem>C1[C@H]2[C@H]3[C@@H]([C@@]4(C(=CC(=O)CC4)CC3)C)CC[C@@]2([C@H](C(COC(C)=O)=O)C1)C</chem>
InChI	1S/C23H32O4/c1-14(24)27-13-21(26)20-7-6-18-17-5-4-15-12-16(25)8-10-22(15,2)19(17)9-11-23(18,20)3/h12,17-20H,4-11,13H2,1-3H3/t17-,18-,19-,20+,22-,23-/m1/s1
InChIKey	VPGRYOFKCNULNK-LCDLLCBDSA-N
Melting Point	157 ° C
Water solubility	8.73 mg/L
log P (octanol-water)	3.08
Atmospheric OH Rate Constant	1.05E-10 cm ³ /molecule-sec
Vapor Pressure	1.32E-08 mm Hg
Henry's Law Constant	1.09E-09 atm-m ³ /mole
Refractive Index	175 ° (C=1, Dioxane)
Storage Temperature	Refrigerator
Merck	2901



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Specifications	Limits
Solubility	H2O: insoluble
Melting Point	157°C



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