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Typical Product Specifications & Properties

11-Deoxycortisol

CAS Number: : 152-58-9

Specifications	Limits
Molecular weight	346.46
EINECS	205-805-2
SMILES	<chem>[C@H]12[C@H]3[C@@H]([C@@]4(C(=CC(=O)CC4)CC3)C)CC[C@@]1([C@](CC2)(C(=O)CO)O)C</chem>
InChI	WHBHBVVOGNECLV-OBQKJFGGSA-N
InChIKey	1S/C21H30O4/c1-19-8-5-14(23)11-13(19)3-4-15-16(19)6-9-20(2)17(15)7-10-21(20,25)18(24)12-22/h11,15-17,22,25H,3-10,12H2,1-2H3/t15-,16+,17+,19+,20+,21+/m1/s1
Atmospheric OH Rate Constant	1.05E-10 cm ³ /molecule-sec
log P (octanol-water)	3.08
Water solubility	15.2 mg/L
Melting Point	215 ° C
Henry's Law Constant	1.58E-06 atm-m ³ /mole
Vapor Pressure	9.49E-12 mm Hg
Density	1.22±0.1 g/cm ³ (20 °C 760 Torr)



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Specifications	Limits
Melting Point	205-208 °C
Flash Point	9?
Refractive Index	120 ° (C=1, Dioxane)
Merck	2932
Storage Temperature	-20°C Freezer



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