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Typical Product Specifications & Properties

Cortisone acetate

CAS Number: : 50-04-4

Specifications	Limits
Molecular weight	402.48
EINECS	200-006-5
SMILES	<chem>C1[C@@]2([C@H]([C@H]3[C@H]([C@@]4(C(=CC(=O)CC4)CC3)C)C1=O)CC[C@@]2(C(COC(C</chem>
InChI	1S/C23H30O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-21(14,2)20(16)18(26)11-22(17,23)3/h10,16-17,20,28H,4-9,11-12t3H3/t16-,17-,20+,21-,22-,23-/m1/s1
InChIKey	ITRJWOMZKQRYTA-XOSMZQINSA-N
Henry's Law Constant	6.51E-14 atm-m ³ /mole
Vapor Pressure	1.10E-12 mm Hg
log P (octanol-water)	2.1
Melting Point	222 ° C
Atmospheric OH Rate Constant	1.08E-10 cm ³ /molecule-sec
Water solubility	20 mg/L
Merck	2539



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Specifications	Limits
Stability	Stable. Incompatible with strong oxidizing agents.
Refractive Index	212 ° (C=1, MeOH)
Melting Point	237-240 °C
Molecular weight	372.50
EINECS	200-275-9
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
Specifications	Limits
Atmospheric OH Rate Constant	1.05E-10 cm ³ /molecule-sec

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Specifications	Limits
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
Solubility	H ₂ O: insoluble
Melting Point	157°C



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