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Typical Product Specifications & Properties

(3 β ,5 β)-3-[(6-deoxy-3-O-methyl- α -L-glucopyranosyl)oxy]-14-hydroxy-19-oxocard-20(22)-enolide

CAS Number: : 1182-87-2

Specifications	Limits
Molecular weight	548.66
EINECS	214-659-9
SMILES	<chem>C1[C@@]2([C@@H]3[C@@H]([C@@]4([C@]([C@@H](C=5COC(C5)=O)CC4)(C)CC3)O)CC[C@@H]2C[C@H](O[C@@H]2[C@@H]([C@H]([C@H](O)[C@@H](O2)C)OC)O)C1)C=O</chem>
InChI	PMT SPAGBAFCORP-HBUONDEYSA-N
InChIKey	1S/C30H44O9/c1-16-24(33)26(36-3)25(34)27(38-16)39-19-6-10-29(15-31)18(13-19)4-5-22-21(29)7-9-28(2)20(8-11-30(22,28)35)17-12-23(32)37-14-17/h12,15-16,18-22,24-27,33-35H,4-11,13-14H2,1-3H3/t16-,18+,19-,20+,21-,22+,24-,25-,26+,27-,28+,29+,30-/m0/s1
log P (octanol-water)	1.05
Melting Point	162.5 ° C
Water solubility	400 mg/L
Henry's Law Constant	2.20E-20 atm-m ³ /mole
Atmospheric OH Rate Constant	1.66E-10 cm ³ /molecule-sec

Vapor Pressure

1.16E-20 mm Hg

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