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Typical Product Specifications & Properties

(3 β ,5 β)-3-[(2,6-dideoxy- β -D-ribohexopyranosyl)oxy]-5,14-dihydroxy-19-oxocard-20(22)-enolide

CAS Number: : 630-64-8

Specifications	Limits
Molecular weight	534.64
EINECS	211-140-9
SMILES	<chem>C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2CC[C@]3(C=O)[C@H]4CC[C@]5(C)[C@H](CC[C@]5(O)[C@@H]4CC[C@]3(O)C2)C6=CC(=O)OC6</chem>
InChI	QBILRDAMJUPXCX-AGAUEGNUSA-N
InChIKey	1S/C29H42O9/c1-16-25(33)22(31)12-24(37-16)38-18-3-8-27(15-30)20-4-7-26(2)19(17-11-23(32)36-14-17)6-10-29(26,35)21(20)5-9-28(27,34)13-18/h11,15-16,18-22,24-25,31,33-35H,3-10,12-14H2,1-2H3/t16-,18+,19-,20+,21-,22+,24+,25-,26-,27+,28+,29+/m1/s1
Vapor Pressure	9.01E-21 mm Hg
log P (octanol-water)	0.3
Water solubility	238 mg/L
Atmospheric OH Rate Constant	1.63E-10 cm ³ /molecule-sec
Henry's Law Constant	5.82E-20 atm-m ³ /mole

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