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Typical Product Specifications & Properties

(3 β ,5 β)-3-[(2,6-dideoxy-3-O-methyl- β -D-ribo-hexopyranosyl)oxy]-5,14,19-trihydroxycard-20(22)-enolide

CAS Number: : 465-84-9

Specifications	Limits
Molecular weight	550.68
EINECS	207-367-8
SMILES	<chem>O1[C@@H](C)[C@@H](O)[C@@H](OC)C[C@@H]1O[C@@H]1C[C@@]2(O)CC[C@@H]3[C@@]4(O)[C@@]4(C)CC[C@@H]3[C@@]2(CO)CC1</chem>
InChI	FCBBZ ANVPISMIM-UHFFFAOYSA-N
InChIKey	1S/C30H46O9/c1-18-25(33)22(36-3)14-24(38-18)39-19-4-10-28(23(32)37-17-27)12-13-30(26,35)21(20)6-11-29(28,34)15-19/h7,9,6,8,10-17H2,1-3H3
log P (octanol-water)	0.56
Vapor Pressure	1.09E-20 mm Hg
Henry's Law Constant	9.81E-19 atm-m ³ /mole
Water solubility	112 mg/L
Atmospheric OH Rate Constant	1.44E-10 cm ³ /molecule-sec