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Typical Product Specifications & Properties

(3β,5β,16β)-3-[(6-deoxy-3-O-methyl-D-galactopyranosyl)oxy]-14,16-dihydroycard-20(22)-enolide

CAS Number: : 595-21-1

Specifications	Limits
EINECS	209-859-8
SMILES	<chem>C[C@@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)O[C@H]2CC[C@]3([C@@H](C2)CC[C@H]4[C@@H]3CC[C@]5([C@@]4C[C@@H]([C@@H]5C6=CC(=O)OC6)O)O)C)O)OC)O</chem>
InChI	CPFNIKYEDJFRAT-RVPZLBNISA-N
InChIKey	1S/C30H46O9/c1-15-24(33)26(36-4)25(34)27(38-15)39-18-7-9-28(2)17(12-18)5-6-20-19(28)8-10-29(3)23(16-11-22(32)37-14-16)21(31)13-30(20,29)35/h11,15,17-21,23-27,31,33-35H,5-10,12-14H2,1-4H3/t15-,17-,18+,19+,20-,21+,23+,24+,25-,26+,27+,28+,29-,30+/m1/s-
log P (octanol-water)	0.59
Water solubility	106 mg/L
Vapor Pressure	9.84E-21 mm Hg
Henry's Law Constant	9.81E-19 atm-m ³ /mole



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