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## Typical Product Specifications & Properties

# (3 $\beta$ ,5 $\beta$ ,16 $\beta$ )-3-[(2,6-dideoxy- $\beta$ -D-ribo-hexopyranosyl)oxy]-14,16-dihydroxycard-20(22)-enolide

CAS Number: : 545-27-7

Specifications	Limits
EINECS	208-887-8
SMILES	<chem>C[C@@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2CC[C@]3([C@H](C2)CC[C@H]4[C@@H]3CC[C@]5([C@@]4(C[C@@H]([C@H]5C6=CC(=O)OC6)O)O)C)C)O</chem>
InChI	IQOYEMCASBGLJD-XQZIZVGLSA-N
InChIKey	1S/C29H44O8/c1-15-26(33)21(30)12-24(36-15)37-18-6-8-27(2)17(11-18)4-5-20-19(27)7-9-28(3)25(16-10-23(32)35-14-16)22(31)13-29(20,28)34/h10,15,17-22,24-26,30-31,33-34H,4-9,11,14H2,1-3H3/t15-,17-,18+,19+,20-,21+,22+,24+,25+,26-,27+,28-,29+/m1/s1
Henry's Law Constant	9.89E-17 atm-m <sup>3</sup> /mole
log P (octanol-water)	1.77
Atmospheric OH Rate Constant	1.35E-10 cm <sup>3</sup> /molecule-sec
Vapor Pressure	4.06E-20 mm Hg
Water solubility	16.2 mg/L

ISO 9001

