

Typical Product Specifications & Properties

(3β,5β)-3-[(6-deoxy-α-L-mannopyranosyl)oxy]-14-hydroxycard-20(22)-enolide

CAS Number: : 508-93-0

Specifications	Limits
Molecular weight	520.65
EINECS	208-088-4
SMILES	<chem>C[C@@H]1O[C@@](C)(O[C@H]2CC[C@@]3(C)[C@H](CC[C@@H]4[C@@H]3CC[C@]5(C)[C@H](CC[C@]45O)C6=CC(=O)OC6)C2)[C@H](O)[C@H](O)[C@H]1O</chem>
InChI	YKTXELZNGPYDJO-GHWIGFALSA-N
InChIKey	1S/C30H46O8/c1-16-24(32)25(33)26(34)29(4,37-16)38-19-7-10-27(2)18(14-19)5-6-22-21(27)8-11-28(3)20(9-12-30(22,28)35)17-13-23(31)36-15-17/h13,16,18-22,24-26,32-35H,5-12,14-15H2,1-4H3/t16-,18+,19-,20+,21-,22+,24-,25+,26+,27-,28+,29-,30-/m0/s1
Atmospheric OH Rate Constant	1.38E-10 cm3/molecule-sec
Vapor Pressure	6.54E-20 mm Hg
Henry's Law Constant	8.38E-17 atm-m3/mole
Water solubility	8.490 mg/L
log P (octanol-water)	2.1