

Typical Product Specifications & Properties

(3β,5β)-3,5,14-trihydroxy-19-oxocard-20(22)-enolide

CAS Number: : 66-28-4

Specifications	Limits
Molecular weight	404.50
EINECS	200-626-6
SMILES	<chem>C[C@]12CC[C@H]3[C@H]([C@]1(CC[C@@H]2C4=CC(=O)OC4)O)CC[C@]5([C@@]3(CC(C5)O)C=O)O</chem>
InChI	ODJLBQGVINUMMR-HZXDTFASSA-N
InChIKey	1S/C23H32O6/c1-20-6-3-17-18(4-8-22(27)11-15(25)2-7-21(17,22,24)23(20,28)9-5-16(20)14-10-19(26)29-12-14/h10,13,15-18,25,27,9,11-12H2,1H3/t15-,16+,17-,18+,20+,21-,22-,23-/m0/s1
log P (octanol-water)	0.64
Melting Point	173 dec ° C
Atmospheric OH Rate Constant	1.10E-10 cm ³ /molecule-sec
Water solubility	816 mg/L
Henry's Law Constant	1.59E-14 atm-m ³ /mole
Vapor Pressure	9.87E-16 mm Hg