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Typical Product Specifications & Properties

(3β,5β,12β)-3,12,14-trihydroxycard-20(22)-enolide

CAS Number: : 1672-46-4

Specifications	Limits
Molecular weight	390.51
EINECS	216-806-2
SMILES	<chem>C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]3[C@@H]2C[C@@H](O)[C@]4(C)[C@H](CC[C@]34O)C5=CC(=O)OC5</chem>
InChI	SHIBSTMRCDJXLN-KCZCNTNESA-N
InChIKey	1S/C23H34O5/c1-21-7-5-15(24)10-14(21)3-4-17-18(21)11-19(25)22(2)16(6-8-23(17,22)27)13-9-20(26)28-12-13/h9,14-19,24-25,27H,3-8,10-12H2,1-2H3/t14-,15+,16-,17-,18+,19-,21+,22+,23+/m1/s1
log P (octanol-water)	1.1
Vapor Pressure	6.69E-15 mm Hg
Water solubility	403 mg/L
Atmospheric OH Rate Constant	8.51E-11 cm ³ /molecule-sec
Henry's Law Constant	2.29E-11 atm-m ³ /mole
Melting Point	222 ° C
Merck	13,3188



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