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Typical Product Specifications & Properties

(3 β ,5 α)-3-[(6-O- β -D-glucopyranosyl- β -D-glucopyranosyl)oxy]-14-hydroxycard-20(22)-enolide

CAS Number: : 20231-81-6

Specifications	Limits
Molecular weight	698.79
EINECS	243-616-7
SMILES	<chem>[C@H]12C[C@H](CC[C@]1(C)[C@@H]1[C@@H](CC2)[C@@]2([C@@]([C@@H](C3=CC(=O)OC3)CC2)(CC1)C)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O1)O)O)CO</chem>
InChI	RIPMDUQTRRLJTE-QHYHXNCWSA-N
InChIKey	1S/C35H54O14/c1-33-8-5-18(46-32-30(28(42)26(40)23(14-37)48-32)49-31-29(43)27(41)25(39)22(13-36)47-31)12-17(33)3-4-21-20(33)6-9-34(2)19(7-10-35(21,34)44)16-11-24(38)45-15-16/h11,17-23,25-32,36-37,39-44H,3-10,12-15H2,1-2H3/t17-,18-,19+,20-,21+,22+,23+,
log P (octanol-water)	-1.630
Melting Point	269 ° C
Atmospheric OH Rate Constant	2.11E-10 cm ³ /molecule-sec



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415 Huguenot Street, New Rochelle, New York 10801

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