Dihydrojatamansin

Inchi: InChI=1S/C19H22O5/c1-5-11(2)18(21)22-15-10-13-14(24-19(15,3)4)8-6-12-7-9-16(20)23
InchiKey: SNISDAOCVKRKNG-UHFFFAOYSA-N
Formula: C19H22O5
SMILES: CCC(C)C(=O)OC1Cc2c(ccc3ccc(=O)oc23)OC1(C)C
Mol. weight [g/mol]: 330.38
CAS: 2221-62-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.02		Crippen Method
logp	3.464		Crippen Method
mcvol	249.540	ml/mol	McGowan Method
rinpol	2561.30		NIST Webbook
rinpol	2561.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2221627&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices