Poligodial + Phe (methyl ester) adduct, (S)

Inchi: InChI=1S/C25H31NO2/c1-24(2)13-8-14-25(3)20-17-26(16-19(20)11-12-22(24)25)21(23(2
InchiKey: XEQFDLHTNOKWPU-IYRGYZHQSA-N
Formula: C25H31NO2
SMILES: COC(=O)C(Cc1ccccc1)n1cc2c(c1)C1(C)CCCC(C)(C)C1C=C2
Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.55		Crippen Method
logp	5.556		Crippen Method
mcvol	311.290	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R163850&Units=SI
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

Legend

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