Poligodial + o-Tyr (ethyl ester) adduct (R,S)

Inchi: InChI=1S/C26H33NO3/c1-5-30-24(29)21(15-18-9-6-7-10-22(18)28)27-16-19-11-12-23-25

InchiKey: IPINMWHPWYBHOL-GMLYINLCSA-N

Formula: C26H33NO3

SMILES: CCOC(=O)C(Cc1ccccc1O)n1cc2c(c1)C1(C)CCCC(C)(C)C1C=C2

Mol. weight [g/mol]: 407.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.51		Crippen Method
logp	5.651		Crippen Method
mcvol	331.250	ml/mol	McGowan Method
rinpol	2985.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R163810&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices