Poligodial + p-Tyr (ethyl ester) adduct (S)

Inchi: InChI=1S/C26H33NO3/c1-5-30-24(29)22(15-18-7-10-20(28)11-8-18)27-16-19-9-12-23-25

InchiKey: OLZYCXZXCDQFBH-SATOSQONSA-N

Formula: C26H33NO3

SMILES: CCOC(=O)C(Cc1ccc(O)cc1)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	3043.00		NIST Webbook
rinpol	3043.00		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=R163865&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.