

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

Latest version available from:

<https://www.chemeo.com/cid/11-028-8/Poligodial-o-Tyr-ethyl-ester-adduct-R-S.pdf>

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