

Poligodial + p-Tyr (ethyl ester) adduct (S), acetylated, # 1

Inchi: InChI=1S/C28H35NO4/c1-6-32-26(31)24(16-20-8-11-22(12-9-20)33-19(2)30)29-17-21-10
InchiKey: NZYKEFNDAKGIFI-CTGOOGPZSA-N
Formula: C28H35NO4
SMILES: CCOC(=O)C(Cc1ccc(OC(C)=O)cc1)n1cc2c(c1)C1(C)CCCC(C)(C)C1C=C2
Mol. weight [g/mol]: 449.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	5.871		Crippen Method
mcvol	361.000	ml/mol	McGowan Method
rinpol	3083.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R163870&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/98-278-6/Poligodial-p-Tyr-ethyl-ester-adduct-S-acetylated-1.pdf>

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