

Poligodial + o-Tyr (ethyl ester) adduct (R,S), acetylated, # 2

Inchi: InChI=1S/C28H35NO4/c1-6-32-26(31)23(16-20-10-7-8-11-24(20)33-19(2)30)29-17-21-12
InchiKey: BETXIFRETZYWON-SYHYUZRHSA-N
Formula: C28H35NO4
SMILES: CCOC(=O)C(Cc1cccc1OC(C)=O)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	2965.00		NIST Webbook
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Sources

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=R163830&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/98-280-3/Poligodial-o-Tyr-ethyl-ester-adduct-R-S-acetylated-2.pdf>

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