

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

Inchi:	InChI=1S/C28H35NO4/c1-6-32-26(31)24(16-20-9-7-10-22(15-20)33-19(2)30)29-17-21-1
InchiKey:	DETHUWXHACXNIF-KBMIILLGSA-N
Formula:	C28H35NO4
SMILES:	CCOC(=O)C(Cc1cccc(OC(C)=O)c1)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	3049.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R163796&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

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<https://www.chemeo.com/cid/98-282-1/Poligodial-m-Tyr-ethyl-ester-adduct-R-S-acetylated-1.pdf>

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