

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

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
rmpol	2957.00		NIST Webbook
rmpol	2957.00		NIST Webbook

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R163825&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R163825&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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<https://www.cheméo.com/cid/98-281-2/Poligodial-o-Tyr-ethyl-ester-adduct-R-S-acetylated-1.pdf>

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