

# 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](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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