

# Trandolapril desethyl - H2O Me (Trandolaprilate - H2O Me)

**Inchi:** InChI=1S/C23H30N2O4/c1-15-21(26)25-18-11-7-6-10-17(18)14-20(25)22(27)24(15)19(2)  
**InchiKey:** BKJUUNRCQXHRMK-TYWFAVLNSA-N  
**Formula:** C23H30N2O4  
**SMILES:** COC(=O)C(CCc1cccc1)N1C(=O)C2CC3CCCCC3N2C(=O)C1C  
**Mol. weight [g/mol]:** 398.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	2.551		Crippen Method
mcvol	309.130	ml/mol	McGowan Method
rinpole	3070.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R550026&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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