

# Tolmetin, methylated

**Inchi:** InChI=1S/C17H19NO3/c1-11-5-7-13(8-6-11)16(19)15-10-9-14(18(15)3)12(2)17(20)21-4/  
**InchiKey:** CAAHZAGZSUNEEN-UHFFFAOYSA-N  
**Formula:** C17H19NO3  
**SMILES:** COC(=O)C(C)c1ccc(C(=O)c2ccc(C)cc2)n1C  
**Mol. weight [g/mol]:** 285.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	2.841		Crippen Method
mcvol	226.160	ml/mol	McGowan Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R201873&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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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