

# Tolmetin, carboxy, bis-methylated

**Inchi:** InChI=1S/C17H17NO5/c1-18-13(10-15(19)22-2)8-9-14(18)16(20)11-4-6-12(7-5-11)17(21)  
**InchiKey:** BQRTZIUBQHQHBD-UHFFFAOYSA-N  
**Formula:** C17H17NO5  
**SMILES:** COC(=O)Cc1ccc(C(=O)c2ccc(C(=O)OC)cc2)n1C  
**Mol. weight [g/mol]:** 315.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	1.758		Crippen Method
mcvol	233.600	ml/mol	McGowan Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R201868&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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