

# Carbamazepine, M(HO-methoxy-ring), AC

**Inchi:** InChI=1S/C18H16N2O4/c1-11(21)24-15-6-8-17-13(10-15)4-3-12-9-14(23-2)5-7-16(12)20  
**InchiKey:** YCSYLXNGAOQDNA-UHFFFAOYSA-N  
**Formula:** C18H16N2O4  
**SMILES:** COc1ccc2c(c1)C=Cc1cc(OC(C)=O)ccc1N2C(N)=O  
**Mol. weight [g/mol]:** 324.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.321		Crippen Method
mcvol	236.640	ml/mol	McGowan Method
rinpole	2420.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R255528&Units=SI>

## 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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