

# N-desmethyacronycine

**Inchi:** InChI=1S/C19H17NO3/c1-19(2)9-8-12-14(23-19)10-15(22-3)16-17(12)20-13-7-5-4-6-11(18)  
**InchiKey:** NEYQKEUFRBPEJP-UHFFFAOYSA-N  
**Formula:** C19H17NO3  
**SMILES:** COc1cc2c(c3[nH]c4cccc4c(=O)c13)C=CC(C)(C)O2  
**Mol. weight [g/mol]:** 307.34

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	3.392		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinsol	2985.00		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=R285717&Units=SI>

## Legend

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

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