

# Neosarranicine

**Inchi:** InChI=1S/C18H27NO5/c1-4-12(3)17(21)24-15-7-9-19-8-6-14(16(15)19)11-23-18(22)13(5)  
**InchiKey:** YMUQRQKYYOWGPN-AXJPLUQKSA-N  
**Formula:** C18H27NO5  
**SMILES:** CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C(=CC)CO)C12  
**Mol. weight [g/mol]:** 337.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.440		Crippen Method
mcvol	264.890	ml/mol	McGowan Method
rinpola	2440.00		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=R178466&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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