

# Clemizole M (hydroxy-methoxy-oxo), acetylated

**Inchi:** InChI=1S/C22H22ClN3O4/c1-14(27)30-20-11-17-18(12-19(20)29-2)26(13-15-5-7-16(23))  
**InchiKey:** OSILSPYOLTZLCJ-UHFFFAOYSA-N  
**Formula:** C22H22ClN3O4  
**SMILES:** COc1cc2c(cc1OC(C)=O)nc(C(=O)N1CCCC1)n2Cc1ccc(Cl)cc1  
**Mol. weight [g/mol]:** 427.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	3.908		Crippen Method
mcvol	304.360	ml/mol	McGowan Method
rinpol	3190.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536273&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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