

# Clemizole, hydroxy-oxo, acetylated

**Inchi:** InChI=1S/C21H20ClN3O3/c1-14(26)28-17-8-9-19-18(12-17)23-20(21(27)24-10-2-3-11-2  
**InchiKey:** MDKMMMDNRYLEISR-UHFFFAOYSA-N  
**Formula:** C21H20ClN3O3  
**SMILES:** CC(=O)Oc1ccc2c(c1)nc(C(=O)N1CCCC1)n2Cc1ccc(Cl)cc1  
**Mol. weight [g/mol]:** 397.86

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	3.899		Crippen Method
mcvol	284.400	ml/mol	McGowan Method
rinpol	3120.00		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=R536268&Units=SI>

## 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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