

# Alprazolam, M (hydroxy-), acetylated

**Inchi:** InChI=1S/C19H15ClN4O2/c1-11-22-23-18-10-21-19(13-3-6-15(7-4-13)26-12(2)25)16-9-1  
**InchiKey:** XEKWYIFSVUGHTL-UHFFFAOYSA-N  
**Formula:** C<sub>19</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>2</sub>  
**SMILES:** CC(=O)Oc1ccc(C2=NCc3nnc(C)n3-c3ccc(Cl)cc32)cc1  
**Mol. weight [g/mol]:** 366.80

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.27		Crippen Method
logp	3.505		Crippen Method
mcvol	256.030	ml/mol	McGowan Method
rinpol	3180.00		NIST Webbook
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## 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=R251977&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  
**rinpol:** Non-polar retention indices

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