

# 4-hydroxy-midazolam

**Inchi:** InChI=1S/C18H13ClFN3O/c1-10-21-9-16-18(24)22-17(12-4-2-3-5-14(12)20)13-8-11(19)6  
**InchiKey:** ZYISITHKPKHPKG-UHFFFAOYSA-N  
**Formula:** C18H13ClFN3O  
**SMILES:** Cc1ncc2n1-c1ccc(Cl)cc1C(c1ccccc1F)=NC2O  
**Mol. weight [g/mol]:** 341.77  
**CAS:** 59468-85-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	3.815		Crippen Method
mcvol	232.160	ml/mol	McGowan Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		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=C59468858&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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