

# Adeptolon, N-desalkyl-hydroxy, acetylated

**Inchi:** InChI=1S/C15H13BrN2O3/c1-10(19)18(13-5-3-12(16)4-6-13)15-8-7-14(9-17-15)21-11(2)  
**InchiKey:** BQBWOOIPJZMCEN-UHFFFAOYSA-N  
**Formula:** C15H13BrN2O3  
**SMILES:** CC(=O)Oc1ccc(N(C(C)=O)c2ccc(Br)cc2)nc1  
**Mol. weight [g/mol]:** 349.18

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	3.454		Crippen Method
mcvol	221.160	ml/mol	McGowan Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535983&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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