

# Adeptolon, N-desalkyl, acetylated

**Inchi:** InChI=1S/C13H11BrN2O/c1-10(17)16(13-4-2-3-9-15-13)12-7-5-11(14)6-8-12/h2-9H,1H3  
**InchiKey:** PIVXAAYMULSLBX-UHFFFAOYSA-N  
**Formula:** C13H11BrN2O  
**SMILES:** CC(=O)N(c1ccc(Br)cc1)c1cccn1  
**Mol. weight [g/mol]:** 291.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	3.529		Crippen Method
mcvol	185.540	ml/mol	McGowan Method
rinpole	2200.00		NIST Webbook
rinpole	2200.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R535978&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpole:** Non-polar retention indices

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