

# 6-Benzylaminopurine, N-acetyl-

**Inchi:** InChI=1S/C14H13N5O/c1-10(20)19(7-11-5-3-2-4-6-11)14-12-13(16-8-15-12)17-9-18-14/  
**InchiKey:** UTPFMWRKSHYOST-UHFFFAOYSA-N  
**Formula:** C14H13N5O  
**SMILES:** CC(=O)N(Cc1ccccc1)c1ncnc2nc[nH]c12  
**Mol. weight [g/mol]:** 267.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	1.424		Crippen Method
mcvol	196.910	ml/mol	McGowan Method
rinpole	2455.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374770&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  
**rinpole:** Non-polar retention indices

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