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/h
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
rinpol	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

Legend

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