

6-Benzylaminopurine, N,N'-di(acetyl)-

Inchi: InChI=1S/C16H15N5O2/c1-11(22)20(8-13-6-4-3-5-7-13)16-14-15(17-9-18-16)19-10-21(1
InchiKey: YERBVWLAWKGISW-UHFFFAOYSA-N
Formula: C16H15N5O2
SMILES: CC(=O)N(Cc1ccccc1)c1ncnc2ncn(C(C)=O)c12
Mol. weight [g/mol]: 309.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	2.039		Crippen Method
mcvol	226.660	ml/mol	McGowan Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374455&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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<https://www.chemeo.com/cid/117-898-6/6-Benzylaminopurine-N-N-di-acetyl.pdf>

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