6-Benzylaminopurine, N,N'-dimethyl-

Inchi: InChI=1S/C14H15N5/c1-18(8-11-6-4-3-5-7-11)14-12-13(15-9-16-14)17-10-19(12)2/h3-7,
InchiKey: BQEXIWGJHQRULH-UHFFFAOYSA-N
Formula: C14H15N5
SMILES: CN(Cc1ccccc1)c1ncnc2ncn(C)c12
Mol. weight [g/mol]: 253.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	2.000		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
rinpol	2413.00		NIST Webbook

Sources

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=U374767&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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