Adenine, N,N'-diacetyl-

Inchi: InChI=1S/C9H9N5O2/c1-5(15)13-8-7-9(11-3-10-8)14(4-12-7)6(2)16/h3-4H,1-2H3,(H,10,1
InchiKey: OWRXXSJEYLRZTG-UHFFFAOYSA-N
Formula: C9H9N5O2
SMILES: CC(=O)Nc1ncnc2c1ncn2C(C)=O
Mol. weight [g/mol]: 219.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	0.445		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
rinpol	1972.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374318&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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