

Adenine, N4-acetyl-

Inchi: InChI=1S/C7H7N5O/c1-4(13)12-7-5-6(9-2-8-5)10-3-11-7/h2-3H,1H3,(H2,8,9,10,11,12,13)
InchiKey: ZURGFCUYILNMNA-UHFFFAOYSA-N
Formula: C7H7N5O
SMILES: CC(=O)Nc1ncnc2[nH]cnc12
Mol. weight [g/mol]: 177.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	-0.171		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
rinpole	1691.00		NIST Webbook
rinpole	1691.00		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=U374319&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/68-913-3/Adenine-N4-acetyl.pdf>

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