

Histamine, N,N'-diacetyl-

Inchi:	InChI=1S/C9H13N3O2/c1-7(13)10-4-3-9-5-12(6-11-9)8(2)14/h5-6H,3-4H2,1-2H3,(H,10,1
InchiKey:	WFVCYFOLCWSCDI-UHFFFAOYSA-N
Formula:	C9H13N3O2
SMILES:	CC(=O)NCCc1cn(C(C)=O)cn1
Mol. weight [g/mol]:	195.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	0.222		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
rinsol	1886.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U374884&Units=SI

Legend

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

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