

1,4-Dimethyl-3-acetyl-4-hydroxy-piperidine

Inchi:	InChI=1S/C9H17NO2/c1-7(11)8-6-10(3)5-4-9(8,2)12/h8,12H,4-6H2,1-3H3
InchiKey:	OOSYAXKYAOWSCZ-UHFFFAOYSA-N
Formula:	C9H17NO2
SMILES:	CC(=O)C1CN(C)CCC1(C)O
Mol. weight [g/mol]:	171.24
CAS:	37994-62-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.47		Crippen Method
logp	0.278		Crippen Method
mcvol	144.230	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37994620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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