

1-Acetyl-4-piperidone

Other names:	N-Acetyl-4-piperidone N-Acetylpiperidone 4-Piperidinone, 1-acetyl-
Inchi:	InChI=1S/C7H11NO2/c1-6(9)8-4-2-7(10)3-5-8/h2-5H2,1H3
InchiKey:	NNFOVLFUGLWWCL-UHFFFAOYSA-N
Formula:	C7H11NO2
SMILES:	CC(=O)N1CCC(=O)CC1
Mol. weight [g/mol]:	141.17
CAS:	32161-06-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	0.198		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
tb	491.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32161061&Units=SI
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

Legend

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

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