

Piperidine, 1-acetyl-

Other names:	Acetic acid, piperidide Ethanone, 1-(1-piperidinyl)- N-Acetylpiperidine 1-Acetylpiperidine N-Acetylpiperidin Acetyl piperidide acetyl piperidine methyl 1-piperidyl ketone
Inchi:	InChI=1S/C7H13NO/c1-7(9)8-5-3-2-4-6-8/h2-6H2,1H3
InchiKey:	KDISMIMTGUMORD-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CC(=O)N1CCCCC1
Mol. weight [g/mol]:	127.18
CAS:	618-42-8

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	1.019		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
rinpol	1205.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1205.00		NIST Webbook
tb	499.20	K	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=C618428&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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