

1-Acetyl-4-piperidinecarboxylic acid

Other names:	1-Acetylpiperidine-4-carboxylic acid 4-Piperidinecarboxylic acid, 1-acetyl-
Inchi:	InChI=1S/C8H13NO3/c1-6(10)9-4-2-7(3-5-9)8(11)12/h7H,2-5H2,1H3,(H,11,12)
InchiKey:	WFCLWJHOKCQYOQ-UHFFFAOYSA-N
Formula:	C8H13NO3
SMILES:	CC(=O)N1CCC(C(=O)O)CC1
Mol. weight [g/mol]:	171.19
CAS:	25503-90-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.27		Crippen Method
logp	0.330		Crippen Method
mcvol	131.710	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25503906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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