L-Proline, 1-acetyl-

Other names:	Proline, 1-acetyl-, L- Acetylproline N-Acetyl-L-proline 1-acetyl-L-proline
Inchi:	InChI=1S/C7H11NO3/c1-5(9)8-4-2-3-6(8)7(10)11/h6H,2-4H2,1H3,(H,10,11)/t6-/m1/s1
InchiKey:	GNMSLDIYJOSUSW-ZCFIWIBFSA-N
Formula:	C7H10NO3
SMILES:	CC(=O)N1CCCC1C(=O)O
Mol. weight [g/mol]:	156.16
CAS:	68-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	0.082		Crippen Method
mcvol	117.620	ml/mol	McGowan Method

Sources

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=C68951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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