

3-Pyrrolidinecarboxylic acid, 1-methyl-5-oxo-

Other names:	1-methyl-5-oxopyrrolidine-3-carboxylic acid 1-methyl-5-oxo-3-pyrrolidinecarboxylic acid
Inchi:	InChI=1S/C6H9NO3/c1-7-3-4(6(9)10)2-5(7)8/h4H,2-3H2,1H3,(H,9,10)
InchiKey:	YHDZDIPQCVCIJS-UHFFFAOYSA-N
Formula:	C6H9NO3
SMILES:	CN1CC(C(=O)O)CC1=O
Mol. weight [g/mol]:	143.14
CAS:	42346-68-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.57		Crippen Method
logp	-0.451		Crippen Method
mcvol	103.530	ml/mol	McGowan Method

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=C42346689&Units=SI

Legend

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

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