2-Pyrrolidone-5-carboxylic acid, N-methyl, methyl ester

Inchi: InChI=1S/C7H11NO3/c1-8-5(7(10)11-2)3-4-6(8)9/h5H,3-4H2,1-2H3
InchiKey: ABAOXDQXQHQRFA-UHFFFAOYSA-N
Formula: C7H11NO3
SMILES: COC(=O)C1CCC(=O)N1C
Mol. weight [g/mol]: 157.17

Physical Properties

Property code	Value	Unit	Source
log10ws	0.03		Crippen Method
logp	-0.220		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
rinpol	1163.30		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333168&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices