Methyl 1-acetylpyrrolidine-2-carboxylate

Inchi: InChI=1S/C8H13NO3/c1-6(10)9-5-3-4-7(9)8(11)12-2/h7H,3-5H2,1-2H3
InchiKey: WCIXKWOJEMZXMK-UHFFFAOYSA-N
Formula: C8H13NO3
SMILES: COC(=O)C1CCCN1C(C)=O
Mol. weight [g/mol]: 171.19
CAS: 18800-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.39		Crippen Method
logp	0.170		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
rinpol	1431.80		NIST Webbook
rinpol	1431.80		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=C18800834&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