Propanoic acid, 3-[N-(2-acetyl-1-pyrrolyl)]

Inchi: InChI=1S/C9H11NO3/c1-7(11)8-3-2-5-10(8)6-4-9(12)13/h2-3,5H,4,6H2,1H3,(H,12,13)
InchiKey: WHAZNHKODRANQY-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: CC(=O)c1cccn1CCC(=O)O
Mol. weight [g/mol]: 181.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Crippen Method
logp	1.165		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
rinpol	1508.00		NIST Webbook

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=R74686&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
rinpol: Non-polar retention indices