Propanoic acid, 3-[N-(2-formyl-5-methyl-1-pyrrolyl)]

Inchi: InChI=1S/C9H11NO3/c1-7-2-3-8(6-11)10(7)5-4-9(12)13/h2-3,6H,4-5H2,1H3,(H,12,13)
InchiKey: NTFDPRYENQKABJ-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: Cc1ccc(C=O)n1CCC(=O)O
Mol. weight [g/mol]: 181.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.084		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		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=R74711&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.