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

Inchi: InChI=1S/C9H11NO4/c11-5-7-1-2-8(6-12)10(7)4-3-9(13)14/h1-2,5,12H,3-4,6H2,(H,13,14

InchiKey: SBILLPGBGOQNIU-UHFFFAOYSA-N

Formula: C9H11NO4

SMILES: O=Cc1ccc(CO)n1CCC(=O)O

Mol. weight [g/mol]: 197.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.63		Crippen Method
logp	0.268		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
rinpol	1700.00		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=R74707&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