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

Inchi: InChI=1S/C8H9NO3/c10-6-7-2-1-4-9(7)5-3-8(11)12/h1-2,4,6H,3,5H2,(H,11,12)
InchiKey: TYZFIRIWLBTRQJ-UHFFFAOYSA-N
Formula: C8H9NO3
SMILES: O=Cc1cccn1CCC(=O)O
Mol. weight [g/mol]: 167.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	0.775		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
rinpol	1450.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R74690&Units=SI
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

Legend

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