

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
rinpola	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
rinpola:	Non-polar retention indices

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