

N-(4-Acetylphenyl)-2,5-dimethylpyrrole

Inchi:	InChI=1S/C14H15NO/c1-10-4-5-11(2)15(10)14-8-6-13(7-9-14)12(3)16/h4-9H,1-3H3
InchiKey:	QYTWQHUEXYLNLA-UHFFFAOYSA-N
Formula:	C14H15NO
SMILES:	CC(=O)c1ccc(-n2c(C)ccc2C)cc1
Mol. weight [g/mol]:	213.28
CAS:	83935-45-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.297		Crippen Method
mcvol	176.450	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C83935459&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/89-918-5/N-4-Acetylphenyl-2-5-dimethylpyrrole.pdf>

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