

# 4-(«alpha»-Ethyl-5-phenyl-1H-pyrrol-3-yl)-pyridine

**Inchi:** InChI=1S/C17H16N2/c1-2-16-15(13-8-10-18-11-9-13)12-17(19-16)14-6-4-3-5-7-14/h3-12  
**InchiKey:** LUHZFCWQVBLSGO-UHFFFAOYSA-N  
**Formula:** C17H16N2  
**SMILES:** CCc1[nH]c(-c2ccccc2)cc1-c1ccncc1  
**Mol. weight [g/mol]:** 248.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	3.824		Crippen Method
mcvol	203.370	ml/mol	McGowan Method
rinpol	1824.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R512648&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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