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
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/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