5-(5-Methyl-2-furyl)-6-methyl-2,3-dihydro-1H-pyrro

Inchi: InChI=1S/C13H15NO/c1-9-8-11-4-3-7-14(11)13(9)12-6-5-10(2)15-12/h5-6,8H,3-4,7H2,1-
InchiKey: LDTMEECXWUGWBZ-UHFFFAOYSA-N
Formula: C13H15NO
SMILES: Cc1ccc(-c2c(C)cc3n2CCC3)o1
Mol. weight [g/mol]: 201.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.30		Crippen Method
logp	3.311		Crippen Method
mcvol	160.100	ml/mol	McGowan Method
ripol	2389.00		NIST Webbook
ripol	2389.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R312057&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.