2-(5-methyl-2-furyl)-1-pyroline

Inchi: InChI=1S/C9H11NO/c1-7-4-5-9(11-7)8-3-2-6-10-8/h4-5H,2-3,6H2,1H3
InchiKey: FCHSRBDFHOMGQE-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: Cc1ccc(C2=NCCC2)o1
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	2.171		Crippen Method
mcvol	118.900	ml/mol	McGowan Method
ripol	1865.00		NIST Webbook
ripol	1865.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R315294&Units=SI

Legend

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

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