2-(5-methyl-2-furyl)-3,4,5,6-tetrahydropyridine

Inchi: InChI=1S/C10H13NO/c1-8-5-6-10(12-8)9-4-2-3-7-11-9/h5-6H,2-4,7H2,1H3
InchiKey: WARIRIKWLUUAPJ-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: Cc1ccc(C2=NCCCC2)o1
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.90		Crippen Method
logp	2.561		Crippen Method
mcvol	132.990	ml/mol	McGowan Method
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315303&Units=SI
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

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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