2-(5-methyl-2-furyl)-3-hydroxy-piperidine

Inchi: InChI=1S/C10H15NO2/c1-7-4-5-9(13-7)10-8(12)3-2-6-11-10/h4-5,8,10-12H,2-3,6H2,1H3
InchiKey: KHCYBVSLKKTRRJ-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: Cc1ccc(C2NCCCC2O)o1
Mol. weight [g/mol]: 181.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.66		Crippen Method
logp	1.373		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
ripol	2169.00		NIST Webbook
ripol	2242.00		NIST Webbook
ripol	2169.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315234&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