2-(2-furyl)-3-hydroxypiperidine

Inchi: InChI=1S/C9H13NO2/c11-7-3-1-5-10-9(7)8-4-2-6-12-8/h2,4,6-7,9-11H,1,3,5H2
InchiKey: KPVVMDIEDRJBAF-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: OC1CCCNC1c1ccco1
Mol. weight [g/mol]: 167.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	1.065		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
ripol	2112.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2112.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315229&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

Latest version available from:
https://www.chemeo.com/cid/98-834-8/2-2-furyl-3-hydroxypiperidine.pdf