2-(5-methyl-2-furyl)pyrrolidine

Inchi: InChI=1S/C9H13NO/c1-7-4-5-9(11-7)8-3-2-6-10-8/h4-5,8,10H,2-3,6H2,1H3
InchiKey: LGGXPKQFJZIICN-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: Cc1ccc(C2CCCN2)o1
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	2.013		Crippen Method
mcvol	123.200	ml/mol	McGowan Method
ripol	1695.00		NIST Webbook
ripol	1695.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315323&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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