5-(5-methyl-2-furyl)-2,3-dihydro-1H-pyrrolizine

Inchi: InChI=1S/C12H13NO/c1-9-4-7-12(14-9)11-6-5-10-3-2-8-13(10)11/h4-7H,2-3,8H2,1H3
InchiKey: SEBQZNHXPWYZSW-UHFFFAOYSA-N
Formula: C12H13NO
SMILES: Cc1ccc(-c2ccc3n2CCC3)o1
Mol. weight [g/mol]: 187.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.82		Crippen Method
logp	3.003		Crippen Method
mcvol	146.010	ml/mol	McGowan Method
ripol	2367.00		NIST Webbook
ripol	2367.00		NIST Webbook

Sources

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=R389027&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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