

2-(2-furyl)-1-pyrroline

Inchi: InChI=1S/C8H9NO/c1-3-7(9-5-1)8-4-2-6-10-8/h2,4,6H,1,3,5H2
InchiKey: RSWIYWDWUHQXIZ-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: c1coc(C2=NCCC2)c1
Mol. weight [g/mol]: 135.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	1.862		Crippen Method
mcvol	104.810	ml/mol	McGowan Method
ripol	1780.00		NIST Webbook
ripol	1780.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R315269&Units=SI>

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/81-327-9/2-2-furyl-1-pyrroline.pdf>

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