

1-(2-furyl)pyrrole

Inchi: InChI=1S/C8H7NO/c1-2-6-9(5-1)8-4-3-7-10-8/h1-7H
InchiKey: PIEDMCUUVINKHS-UHFFFAOYSA-N
Formula: C8H7NO
SMILES: c1coc(-n2cccc2)c1
Mol. weight [g/mol]: 133.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	2.070		Crippen Method
mcvol	100.510	ml/mol	McGowan Method
ripol	1823.00		NIST Webbook
ripol	1823.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R321561&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/88-252-5/1-2-furyl-pyrrole.pdf>

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