

Pyrrolidine, 1-furfuryl

Inchi: InChI=1S/C9H11NO2/c11-9(8-4-3-7-12-8)10-5-1-2-6-10/h3-4,7H,1-2,5-6H2
InchiKey: YBHIXZDADAIOMV-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: O=C(c1ccco1)N1CCCC1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.08		Crippen Method
logp	1.516		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62435&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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