

1-(5'-methylfurfuryl)pyrrolidine

Other names: Pyrrolidine, 1-(5-methylfurfuryl)
Inchi: InChI=1S/C10H15NO/c1-9-4-5-10(12-9)8-11-6-2-3-7-11/h4-5H,2-3,6-8H2,1H3
InchiKey: IETSEKPJTAMXGM-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: Cc1ccc(CN2CCCC2)o1
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.70		Crippen Method
logp	2.184		Crippen Method
mcvol	137.290	ml/mol	McGowan Method
rinpol	1225.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1226.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1600.00		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=U366039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

ripol: Polar retention indices

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