

1-(5'-methyلفurfuryl)pyrrolidine

Other names:	Pyrrolidine, 1-(5-methyلفurfuryl)
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	1226.00		NIST Webbook
rinpol	1225.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1600.00		NIST Webbook

Sources

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/ci990307l
Crippen Method:	https://www.chemeo.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

ripol:

Polar retention indices

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