

1[5'-(hydroxymethyl)furfuryl]pyrrolidine

Other names:	1-(5-(hydroxymethyl)furfuryl)pyrrolidine
Inchi:	InChI=1S/C10H15NO2/c12-8-10-4-3-9(13-10)7-11-5-1-2-6-11/h3-4,12H,1-2,5-8H2
InchiKey:	POLAFJCRVYXYDM-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	<chem>OCc1ccc(CN2CCCC2)o1</chem>
Mol. weight [g/mol]:	181.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	1.368		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
ripol	2375.00		NIST Webbook
ripol	2375.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366033&Units=SI
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

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/90-948-0/1-5-hydroxymethyl-furfuryl-pyrrolidine.pdf>

Generated by Cheméo on 2024-04-23 16:32:49.868007533 +0000 UTC m=+16179218.788584845.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.