Pyrrole, 1-(5-methylfurfuryl)

Other names:	1-(5-methylfurfuryl)-pyrrole
Inchi:	InChI=1S/C10H11NO/c1-9-4-5-10(12-9)8-11-6-2-3-7-11/h2-7H,8H2,1H3
InchiKey:	CAHIUMOBCXFSCC-UHFFFAOYSA-N
Formula:	C10H11NO
SMILES:	Cc1ccc(Cn2cccc2)o1
Mol. weight [g/mol]:	161.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	2.438		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
rinpol	1247.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1247.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1885.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

ripol: Polar retention indices

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https://www.chemeo.com/cid/85-996-3/Pyrrole-1-5-methylfurfuryl.pdf

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