

1,3,5-trimethylpyrrole

Inchi:	InChI=1S/C7H11N/c1-6-4-7(2)8(3)5-6/h4-5H,1-3H3
InchiKey:	JAPNKJDKITTYLO-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	Cc1cc(C)n(C)c1
Mol. weight [g/mol]:	109.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	1.642		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rmpol	976.00		NIST Webbook
rmpol	976.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R346060&Units=SI

Legend

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

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<https://www.cheméo.com/cid/16-139-0/1-3-5-trimethylpyrrole.pdf>

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