

2,3,4-Trimethylpyrrole

Other names:	2,3,4-trimethyl-1H-pyrrole
Inchi:	InChI=1S/C7H11N/c1-5-4-8-7(3)6(5)2/h4,8H,1-3H3
InchiKey:	WTMJHBZSSSDBFQ-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	Cc1c[nH]c(C)c1C
Mol. weight [g/mol]:	109.17
CAS:	3855-78-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.458		Crippen Method
mcvol	100.010	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3855785&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/16-391-0/2-3-4-Trimethylpyrrole.pdf>

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