

1H-Pyrrole, 3-methyl-2-propyl

Inchi:	InChI=1S/C8H13N/c1-3-4-8-7(2)5-6-9-8/h5-6,9H,3-4H2,1-2H3
InchiKey:	PBGHXNWNXGNGDD-UHFFFAOYSA-N
Formula:	C8H13N
SMILES:	CCc1[nH]ccc1C
Mol. weight [g/mol]:	123.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.794		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpole	1162.00		NIST Webbook
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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=R129563&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/53-651-0/1H-Pyrrole-3-methyl-2-propyl.pdf>

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