2-ethyl-3-methylpyrrole

Inchi:	InChI=1S/C7H11N/c1-3-8-6-4-5-7(8)2/h4-6H,3H2,1-2H3
InchiKey:	WBSWPBIIIRQMFK-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	CCn1cccc1C
Mol. weight [g/mol]:	109.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	1.816		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236601&Units=SI

Legend

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

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