1H-Pyrrole, 2-ethyl-5-methyl

Inchi:	InChI=1S/C7H11N/c1-3-7-5-4-6(2)8-7/h4-5,8H,3H2,1-2H3
InchiKey:	GXSYXPDGMUORDR-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	CCc1ccc(C)[nH]1
Mol. weight [g/mol]:	109.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.404		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook

Sources

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=R129558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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