

7-ethyl-N-methylindole

Inchi:	InChI=1S/C11H13N/c1-3-9-5-4-6-10-7-8-12(2)11(9)10/h4-8H,3H2,1-2H3
InchiKey:	PNBISRBPZVZDNJ-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	CCc1cccc2ccn(C)c12
Mol. weight [g/mol]:	159.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	2.741		Crippen Method
mcvol	136.910	ml/mol	McGowan Method
rinpola	1481.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R408549&Units=SI
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

Legend

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

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