

5-Hydroxyindole, N-methyl-, methyl ether

Inchi:	InChI=1S/C10H11NO/c1-11-6-5-8-7-9(12-2)3-4-10(8)11/h3-7H,1-2H3
InchiKey:	HQNPKVBTBJUMTR-UHFFFAOYSA-N
Formula:	C10H11NO
SMILES:	COc1ccc2c(ccn2C)c1
Mol. weight [g/mol]:	161.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	2.187		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
rinpol	1556.70		NIST Webbook

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=U333384&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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<https://www.chemeo.com/cid/29-940-6/5-Hydroxyindole-N-methyl-methyl-ether.pdf>

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