

5-Methoxy-4-methoxymethyl-2-methyl-1H-indole

Inchi:	InChI=1S/C12H15NO2/c1-8-6-9-10(7-14-2)12(15-3)5-4-11(9)13-8/h4-6,13H,7H2,1-3H3
InchiKey:	OQSVAFMVCFOGM-UHFFFAOYSA-N
Formula:	C12H15NO2
SMILES:	COCc1c(OC)ccc2[nH]c(C)cc12
Mol. weight [g/mol]:	205.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.149		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
rinpole	1800.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586213&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
rinpole:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/23-552-3/5-Methoxy-4-methoxymethyl-2-methyl-1H-indole.pdf>

Generated by Cheméo on 2024-04-23 11:20:00.658042916 +0000 UTC m=+16160449.578620232.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.