

4-Hydroxymethyl-2-methyl-1H-indole

Inchi:	InChI=1S/C10H11NO/c1-7-5-9-8(6-12)3-2-4-10(9)11-7/h2-5,11-12H,6H2,1H3
InchiKey:	UTVNVUWKZNLNT-UHFFFAOYSA-N
Formula:	C10H11NO
SMILES:	Cc1cc2c(CO)cccc2[nH]1
Mol. weight [g/mol]:	161.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	1.487		Crippen Method
mcvol	128.690	ml/mol	McGowan Method
rinpola	1750.00		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=R586184&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
rinpola:	Non-polar retention indices

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