

1H-Indole, 6-methoxy-

Other names:	Indole, 6-methoxy- 6-Methoxyindole 6-Methoxy-1H-indole
Inchi:	InChI=1S/C9H9NO/c1-11-8-3-2-7-4-5-10-9(7)6-8/h2-6,10H,1H3
InchiKey:	QJRWYBIKLXNYLF-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	COc1ccc2cc[nH]c2c1
Mol. weight [g/mol]:	147.17
CAS:	3189-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.695		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
rinpol	1574.00		NIST Webbook
rinpol	1563.00		NIST Webbook
ripol	2826.00		NIST Webbook
ripol	2807.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C3189137&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
ripol: Polar retention indices

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<https://www.chemeo.com/cid/58-668-7/1H-Indole-6-methoxy.pdf>

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