

Indole, 5-methoxy, TMS

Inchi:	InChI=1S/C12H17NOSi/c1-14-11-5-6-12-10(9-11)7-8-13(12)15(2,3)4/h5-9H,1-4H3
InchiKey:	ASZNBXCIENWVIC-UHFFFAOYSA-N
Formula:	C12H17NOSi
SMILES:	COc1ccc2c(ccn2[Si](C)(C)C)c1
Mol. weight [g/mol]:	219.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Crippen Method
logp	3.333		Crippen Method
rinpol	1660.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R529181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/13-071-8/Indole-5-methoxy-TMS.pdf>

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