

Indole-3-carboxaldehyde, 5-methoxy, TMS

Inchi: InChI=1S/C13H17NO2Si/c1-16-11-5-6-13-12(7-11)10(9-15)8-14(13)17(2,3)4/h5-9H,1-4H
InchiKey: PIMBGPYOZOVPSJ-UHFFFAOYSA-N
Formula: C13H17NO2Si
SMILES: COc1ccc2c(c1)c(C=O)cn2[Si](C)(C)C
Mol. weight [g/mol]: 247.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	3.145		Crippen Method
rinpol	2125.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529121&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/10-655-3/Indole-3-carboxaldehyde-5-methoxy-TMS.pdf>

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