

Indole, 3-(3-oxobutyl), 5-methoxy, TMS

Inchi: InChI=1S/C16H23NO2Si/c1-12(18)6-7-13-11-17(20(3,4)5)16-9-8-14(19-2)10-15(13)16/h
InchiKey: CDKPJASBYKFEDN-UHFFFAOYSA-N
Formula: C16H23NO2Si
SMILES: COc1ccc2c(c1)c(CCC(C)=O)cn2[Si](C)(C)C
Mol. weight [g/mol]: 289.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	3.854		Crippen Method
rinpol	2110.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529092&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/13-689-3/Indole-3-3-oxobutyl-5-methoxy-TMS.pdf>

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