

Indole-3-butyric acid, mono-TMS

Inchi: InChI=1S/C15H21NO2Si/c1-19(2,3)18-15(17)10-6-7-12-11-16-14-9-5-4-8-13(12)14/h4-5,
InchiKey: JYXWAJZZQQWQEA-UHFFFAOYSA-N
Formula: C15H21NO2Si
SMILES: C[Si](C)(C)OC(=O)CCCc1c[nH]c2ccccc12
Mol. weight [g/mol]: 275.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	3.387		Crippen Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401102&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/121-539-9/Indole-3-butyric-acid-mono-TMS.pdf>

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