

Indole, 3-(2-hexanoyloxyethyl), 5-methoxy, TMS

Inchi: InChI=1S/C20H31NO3Si/c1-6-7-8-9-20(22)24-13-12-16-15-21(25(3,4)5)19-11-10-17(23-2)
InchiKey: BYHINIGGMKVPIR-UHFFFAOYSA-N
Formula: C20H31NO3Si
SMILES: CCCCCC(=O)OCCc1cn([Si](C)(C)C)c2ccc(OC)cc12
Mol. weight [g/mol]: 361.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	4.999		Crippen Method
rinpol	2480.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529032&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/33-743-0/Indole-3-2-hexanoyloxyethyl-5-methoxy-TMS.pdf>

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