

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

Inchi: InChI=1S/C19H29NO3Si/c1-6-7-8-19(21)23-12-11-15-14-20(24(3,4)5)18-10-9-16(22-2)1
InchiKey: ADJGKZYDZHDETI-UHFFFAOYSA-N
Formula: C19H29NO3Si
SMILES: CCCCC(=O)OCCc1cn([Si](C)(C)C)c2ccc(OC)cc12
Mol. weight [g/mol]: 347.52

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.49 | | Crippen Method |
| logp | 4.609 | | Crippen Method |
| rinpol | 2385.00 | | NIST Webbook |
| rinpol | 2385.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529052&Units=SI>

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/44-442-2/Indole-3-2-pentanoyloxyethyl-5-methoxy-TMS.pdf>

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