

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

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| Inchi: | InChI=1S/C18H27NO3Si/c1-6-7-18(20)22-11-10-14-13-19(23(3,4)5)17-9-8-15(21-2)12-1 |
| InchiKey: | JASQWQBDOUHBN-UHFFFAOYSA-N |
| Formula: | C18H27NO3Si |
| SMILES: | CCCC(=O)OCCc1cn([Si](C)(C)C)c2ccc(OC)cc12 |
| Mol. weight [g/mol]: | 333.50 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.07 | | Crippen Method |
| logp | 4.219 | | Crippen Method |
| rinpol | 2330.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R529012&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.cheméo.com/cid/25-391-0/Indole-3-2-butanoyloxyethyl-5-methoxy-TMS.pdf>

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