

3-Indolepropionic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C20H29NO4Si/c1-7-24-19(23)21-14-15(16-10-8-9-11-17(16)21)12-13-18(22)20
InchiKey: JPCOXSHSLQDXIF-UHFFFAOYSA-N
Formula: C20H29NO4Si
SMILES: CCOC(=O)n1cc(CCC(=O)O[Si](C)(C)C(C)(C)C)c2ccccc21
Mol. weight [g/mol]: 375.53

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.05 | | Crippen Method |
| logp | 5.127 | | Crippen Method |
| rinpol | 2282.00 | | NIST Webbook |
| rinpol | 2282.00 | | 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=R563552&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/49-392-3/3-Indolepropionic-acid-ethoxycarbonylated-TBDMS.pdf>

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