

3-(2-Hydroxyethyl)indole, bromomethyl dimethylsilyl ether

Inchi: InChI=1S/C13H18BrNOSi/c1-17(2,10-14)16-8-7-11-9-15-13-6-4-3-5-12(11)13/h3-6,9,15H
InchiKey: PONCQTXDXSGHSI-UHFFFAOYSA-N
Formula: C13H18BrNOSi
SMILES: C[Si](C)(CBr)OCCc1c[nH]c2cccc12
Mol. weight [g/mol]: 312.28

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.21 | | Crippen Method |
| logp | 3.384 | | Crippen Method |
| rinpol | 2221.00 | | NIST Webbook |
| rinpol | 2221.00 | | 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=U375743&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/61-723-1/3-2-Hydroxyethyl-indole-bromomethyl dimethylsilyl-ether.pdf>

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