

Timolol, TBDMS

Inchi: InChI=1S/C18H36N4O3SSi/c1-14(2)19-12-15(25-27(6,7)18(3,4)5)13-24-17-16(20-26-21-18)
InchiKey: DCGFAXJUVDXAJO-UHFFFAOYSA-N
Formula: C18H36N4O3SSi
SMILES: CC(C)NCC(COc1nsnc1N1CCOCC1)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 416.65

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.76 | | Crippen Method |
| logp | 3.142 | | Crippen Method |
| rinpol | 2511.00 | | NIST Webbook |
| rinpol | 2511.00 | | 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=R435388&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/23-981-7/Timolol-TBDMS.pdf>

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