

Penbutolol, N-ethoxycarbonylated, TMS

Inchi: InChI=1S/C24H41NO4Si/c1-8-27-23(26)25(24(2,3)4)17-20(29-30(5,6)7)18-28-22-16-12-11
InchiKey: YIQOJHZWGOVHQM-UHFFFAOYSA-N
Formula: C24H41NO4Si
SMILES: CCOC(=O)N(CC(COc1ccccc1C1CCCC1)O[Si](C)(C)C)C(C)C
Mol. weight [g/mol]: 435.67

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.30 | | Crippen Method |
| logp | 6.200 | | Crippen Method |
| rinpol | 2492.30 | | NIST Webbook |
| rinpol | 2492.30 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R435259&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/84-143-0/Penbutolol-N-ethoxycarbonylated-TMS.pdf>

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