

Metipranolol, PFB-TMS

Inchi: InChI=1S/C27H34F5NO5Si/c1-13(2)33(27(35)20-21(28)23(30)25(32)24(31)22(20)29)11-
InchiKey: HCUINBYOODQVTA-UHFFFAOYSA-N
Formula: C27H34F5NO5Si
SMILES: CC(=O)Oc1c(C)cc(OCC(CN(C(=O)c2c(F)c(F)c(F)c(F)c2F)C(C)C)O[Si](C)(C)C)c(C)c1C
Mol. weight [g/mol]: 575.64

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.66 | | Crippen Method |
| logp | 6.382 | | Crippen Method |
| rinpol | 2844.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R175056&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/77-248-2/Metipranolol-PFB-TMS.pdf>

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