Carteolol, PFB-TMS

Inchi: InChI=1S/C23H31F7N2O4Si/c1-20(2,3)32(19(34)21(24,25)22(26,27)23(28,29)30)12-14(
InchiKey: GIPYLOMCALTREM-UHFFFAOYSA-N
Formula: C23H31F7N2O4Si
SMILES: CC(C)(C)N(CC(COc1cccc2c1CCC(=O)N2)O[Si](C)(C)C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 560.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	5.630		Crippen Method
rinpol	3159.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319147&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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