(-)-Bunolol, PFB-TMS

Inchi: InChI=1S/C27H32F5NO4Si/c1-27(2,3)33(26(35)20-21(28)23(30)25(32)24(31)22(20)29)1
InchiKey: DZGLEEKVLFHXAV-UHFFFAOYSA-N
Formula: C27H32F5NO4Si
SMILES: CC(C)(C)N(CC(COc1cccc2c1CCCC2=O)O[Si](C)(C)C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 557.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	6.441		Crippen Method
rinpol	2961.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R175016&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