(-)-Bunolol methoxime, PFB-TMS

Inchi: InChI=1S/C28H35F5N2O4Si/c1-28(2,3)35(27(36)21-22(29)24(31)26(33)25(32)23(21)30)
InchiKey: LZXPQHKVFXZXLX-ALQBTCKLSA-N
Formula: C28H35F5N2O4Si
SMILES: CON=C1CCCc2c(OCC(CN(C(=O)c3c(F)c(F)c(F)c(F)c3F)C(C)(C)C)O[Si](C)(C)C)cccc21
Mol. weight [g/mol]: 586.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	6.609		Crippen Method
rinpol	3051.00		NIST Webbook
rinpol	3051.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R175001&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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