p-Synephrine, DTFMB-TMS

Other names: p-Synephrine, N-DTFMB-TMS
Inchi: InChI=1S/C24H31F6NO3Si2/c1-31(22(32)17-12-18(23(25,26)27)14-19(13-17)24(28,29)3
InchiKey: FTLDSFURVGIGJP-UHFFFAOYSA-N
Formula: C24H31F6NO3Si2
SMILES: CN(CC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)cc1)C(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 551.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	7.603		Crippen Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54214&Units=SI

Legend

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