Adrenaline, DTFMB-TBDMS

Inchi: InChI=1S/C36H57F6NO4Si3/c1-32(2,3)48(11,12)45-28-18-17-24(21-29(28)46-49(13,14)
InchiKey: UMDBQTBNTLUKHK-UHFFFAOYSA-N
Formula: C36H57F6NO4Si3
SMILES: CN(CC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1)C(=O
Mol. weight [g/mol]: 766.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	12.327		Crippen Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		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=R54068&Units=SI

Legend

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