m-Synephrine, DTFMB-TBDMS

Inchi: InChI=1S/C30H43F6NO3Si2/c1-27(2,3)41(8,9)39-24-14-12-13-20(17-24)25(40-42(10,11)
InchiKey: XWUZJJWTFJILDD-UHFFFAOYSA-N
Formula: C30H43F6NO3Si2
SMILES: CN(CC(O[Si](C)(C)C(C)(C)C)c1cccc(O[Si](C)(C)C(C)(C)C)c1)C(=O)c1cc(C(F)(F)F)cc(C(
Mol. weight [g/mol]: 635.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.23		Crippen Method
logp	9.943		Crippen Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54143&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