Dopamine, DTFMB-TBDMS

Inchi: InChI=1S/C29H41F6NO3Si2/c1-26(2,3)40(7,8)38-23-12-11-19(15-24(23)39-41(9,10)27(4
InchiKey: JMLSSKPCWIHELM-UHFFFAOYSA-N
Formula: C29H41F6NO3Si2
SMILES: CC(C)(C)[Si](C)(C)Oc1ccc(CCNC(=O)c2cc(C(F)(F)F)cc(C(F)(F)F)c2)cc1O[Si](C)(C)C(C)
Mol. weight [g/mol]: 621.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	9.465		Crippen Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R54107&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