Dopamine, PFB-TMS

Inchi: InChI=1S/C21H26F5NO3Si2/c1-31(2,3)29-13-8-7-12(11-14(13)30-32(4,5)6)9-10-27-21(2
InchiKey: FMPNZWUCJCQBJZ-UHFFFAOYSA-N
Formula: C21H26F5NO3Si2
SMILES: C[Si](C)(C)Oc1ccc(CCNC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 491.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	5.782		Crippen Method
rinpol	2184.00		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=R305767&Units=SI

Legend

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