Normetanephrine, PFB-TMS

Inchi: InChI=1S/C22H28F5NO4Si2/c1-30-14-10-12(8-9-13(14)31-33(2,3)4)15(32-34(5,6)7)11-2
InchiKey: DHYALGQTRNCMGU-UHFFFAOYSA-N
Formula: C22H28F5NO4Si2
SMILES: COc1cc(C(CNC(=O)c2c(F)c(F)c(F)c(F)c2F)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 521.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	5.927		Crippen Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305787&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