Benzeneethanamine, N-[(pentafluorophenyl)methylene]-«beta»-[(trimet

Other names: 2-Hydroxy-2-phenylethylamine, PFB-imine, TMS
Inchi: InChI=1S/C18H18F5NOSi/c1-26(2,3)25-13(11-7-5-4-6-8-11)10-24-9-12-14(19)16(21)18(
InchiKey: OCLLTNUKNVMOOC-UHFFFAOYSA-N
Formula: C18H18F5NOSi
SMILES: C[Si](C)(C)OC(CN=Cc1c(F)c(F)c(F)c(F)c1F)c1ccccc1
Mol. weight [g/mol]: 387.42
CAS: 55334-63-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	5.394		Crippen Method
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334639&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