Benzeneethanamine, 4-methoxy-N-[(pentafluorophenyl)methylene]-3-[(t

Other names: 2-(3-Hydroxy-4-methoxyphenyl)ethylamine, PFB-imine, TMS
Inchi: InChI=1S/C19H20F5NO2Si/c1-26-13-6-5-11(9-14(13)27-28(2,3)4)7-8-25-10-12-15(20)17
InchiKey: XSRGUHNJXDKJOO-UHFFFAOYSA-N
Formula: C19H20F5NO2Si
SMILES: COc1ccc(CCN=Cc2c(F)c(F)c(F)c(F)c2F)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 417.45
CAS: 55556-73-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	5.266		Crippen Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55556735&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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