Benzeneethanamine, N-[(pentafluorophenyl)methylene]-3,4-bis[(trimeth

Other names: N-(Pentafluorobenzylidene)-3,4-bis(trimethylsiloxy) phenylethylamine
Dopamine, PFB-imine, TMS

Inchi: InChI=1S/C21H26F5NO2Si2/c1-30(2,3)28-15-8-7-13(11-16(15)29-31(4,5)6)9-10-27-12-1

InchiKey: XLVPTHFHTULEAF-UHFFFAOYSA-N

Formula: C21H26F5NO2Si2

SMILES: C[Si](C)(C)Oc1ccc(CCN=Cc2c(F)c(F)c(F)c(F)c2F)cc1O[Si](C)(C)C

Mol. weight [g/mol]: 475.60

CAS: 50314-21-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	6.471		Crippen Method
rinpol	2198.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2198.00		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=C50314211&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices