Benzeneethanamine, N-[(pentafluorophenyl)methylene]-«beta»,4-bis[(tr

Other names: Octopamine, PFB-imine, TMS

Inchi: InChI=1S/C21H26F5NO2Si2/c1-30(2,3)28-14-9-7-13(8-10-14)16(29-31(4,5)6)12-27-11-1

InchiKey: LKJPSAODMMZLQD-UHFFFAOYSA-N

Formula: C21H26F5NO2Si2

SMILES: C[Si](C)(C)Oc1ccc(C(CN=Cc2c(F)c(F)c(F)c(F)c2F)O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 475.60

CAS: 55429-85-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	6.607		Crippen Method
rinpol	2159.00		NIST Webbook
rinpol	2159.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55429851&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