Phenylethanolamine triTMS

Other names: Tyramine, tris-TMS
Inchi: InChI=1S/C17H35NOSi3/c1-20(2,3)18(21(4,5)6)15-14-16-10-12-17(13-11-16)19-22(7,8)9
InchiKey: WDQQWJKBIMOZAK-UHFFFAOYSA-N
Formula: C17H35NOSi3
SMILES: C[Si](C)(C)Oc1ccc(CCN([Si](C)(C)C)[Si](C)(C)C)cc1
Mol. weight [g/mol]: 353.72
CAS: 68595-84-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.53		Crippen Method
logp	5.415		Crippen Method
rinpol	1922.00		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=C68595846&Units=SI

Legend

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