

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)
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
rinsol	1922.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/93-102-5/Phenylethanolamine-triTMS.pdf>

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