

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]:	353.73

Physical Properties

Property code	Value	Unit	Source
hvap	66.82	kJ/mol	Cheméo Relay (1.0)
logp	5.415		Crippen Method
rinpol	1922.00		NIST Webbook
rinpol	1922.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68595846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/93-102-5/PHENYLETHANOLAMINE-TRITMS.pdf>

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