Histamine, N,N,N'-tris(trimethylsilyl)-

Other names:	Bis(trimethylsilyl)pyrrol2-[1-(trimethylsilyl)-1H-imidazol-4-yl]ethylmorphoamine
	Histamine, tris-TMS
	Histamine, 3tms derivative
Inchi:	InChI=1S/C14H33N3Si3/c1-18(2,3)16-12-14(15-13-16)10-11-17(19(4,5)6)20(7,8)9/h12-1
InchiKey:	JHBJMCFUYLNCSZ-UHFFFAOYSA-N
Formula:	C14H33N3Si3
SMILES:	C[Si](C)(C)N(CCc1cn([Si](C)(C)C)cn1)[Si](C)(C)C
Mol. weight [g/mol]:	327.69

Physical Properties

Property code	Value	Unit	Source
log10ws	2.44		Crippen Method
logp	4.080		Crippen Method
rinpol	1870.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1880.30		NIST Webbook
rinpol	1870.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333770&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

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