

Histamine, N,N'-bis(tert-butyldimethylsilyl)-

Other names:	[tert-Butyl(dimethyl)silyl](2-pyrrol1-[tert-butyl(dimethyl)silyl]-1H-imidazol-4-ylmorphoethyl) Histamine, 2tbdms derivative
Inchi:	InChI=1S/C17H37N3Si2/c1-16(2,3)21(7,8)19-12-11-15-13-20(14-18-15)22(9,10)17(4,5)6
InchiKey:	OQZFYIDVXMIKJJ-UHFFFAOYSA-N
Formula:	C17H37N3Si2
SMILES:	CC(C)(C)[Si](C)(C)NCCc1cn([Si](C)(C)C(C)(C)C)cn1
Mol. weight [g/mol]:	339.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	4.874		Crippen Method
rinpol	2093.00		NIST Webbook
rinpol	2093.00		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=U333768&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/16-330-7/Histamine-N-N-bis-tert-butyldimethylsilyl.pdf>

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