Histidine, N,N,O-3TMS

Other names:	Histidine, N,1-bis-(trimethylsilyl)-, trimethylsilyl ester
	N,N',o-Tris-(trimethylsilyl)histidine
	Imidazole-4-alanine, N,1-bis(trimethylsilyl)-, trimethylsilyl ester, L-
	Histidine, tri-TMS
	HIS, tris-TMS
	His, TMS
	Histidine, TMS
Inchi:	InChI=1S/C15H33N3O2Si3/c1-21(2,3)17-14(15(19)20-23(7,8)9)10-13-11-18(12-16-13)22
InchiKey:	MEFLGORIMZDUEG-UHFFFAOYSA-N
Formula:	C15H33N3O2Si3
SMILES:	C[Si](C)(C)NC(Cc1cn([Si](C)(C)C)cn1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	371.70

Physical Properties

Property code	Value	Unit	Source
log10ws	2.43		Crippen Method
logp	3.280		Crippen Method
rinpol	1916.60		NIST Webbook
rinpol	1921.05		NIST Webbook
rinpol	1942.25		NIST Webbook
rinpol	1941.81		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1920.38		NIST Webbook
rinpol	1947.08		NIST Webbook
ripol	2293.85		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=C17908257&Units=SI

Legend

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

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