Histidine, MTH-TMS

Inchi:	InChI=1S/C14H26N4OSSi2/c1-17-13(19-22(5,6)7)12(16-14(17)20)8-11-9-18(10-15-11)2
InchiKey:	MWWQIGFREQFWDG-UHFFFAOYSA-N
Formula:	C14H26N4OSSi2
SMILES:	Cn1c(O[Si](C)(C)C)c(Cc2cn([Si](C)(C)C)cn2)[nH]c1=S
Mol. weight [g/mol]:	354.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	3.285		Crippen Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		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=R525441&Units=SI

Legend

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

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