N-Acetylhistamine, TMS

Inchi: InChI=1S/C14H27N3O3Si2/c1-11(18)16-13(14(19)20-22(5,6)7)8-12-9-17(10-15-12)21(2,
InchiKey: CYRMTJAGQABXKW-UHFFFAOYSA-N
Formula: C14H27N3O3Si2
SMILES: CC(=O)NC(Cc1cn([Si](C)(C)C)cn1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 341.55

Physical Properties

Property code	Value	Unit	Source
log10ws	1.12		Crippen Method
logp	1.991		Crippen Method
rinpol	1809.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R95121&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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