

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/ci9903071

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/41-444-3/N-Acetylhistamine-TMS.pdf>

Generated by Cheméo on 2024-04-26 20:00:54.582769886 +0000 UTC m=+16450903.503347202.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.