

Histamine, N,N,N'-tris(trimethylsilyl)-

Other names: Bis(trimethylsilyl)pyrrol2-[1-(trimethylsilyl)-1H-imidazol-4-yl]ethylmorphoamine
Histamine, tris-TMS
Histamine, 3tms derivative

Inchi: InChI=1S/C14H33N3Si3/c1-18(2,3)16-12-14(15-13-16)10-11-17(19(4,5)6)20(7,8)9/h12-1

InchiKey: JHBJMCFUYLNCSZ-UHFFFAOYSA-N

Formula: C14H33N3Si3

SMILES: C[Si](C)(C)N(Cc1cn([Si](C)(C)C)cn1)[Si](C)(C)C

Mol. weight [g/mol]: 327.69

Physical Properties

Property code	Value	Unit	Source
log10ws	2.44		Crippen Method
logp	4.080		Crippen Method
rinpol	1870.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1880.30		NIST Webbook
rinpol	1870.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333770&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/53-036-3/Histamine-N-N-N-tris-trimethylsilyl.pdf>

Generated by Cheméo on 2024-04-19 19:19:51.83387103 +0000 UTC m=+15843640.754448343.

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