

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525441&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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/37-146-9/Histidine-MTH-TMS.pdf>

Generated by Cheméo on 2024-04-24 02:25:17.764779407 +0000 UTC m=+16214766.685356719.

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