

«epsilon»-Methylthiocarbamyl lysine, MTH-TMS

Inchi: InChI=1S/C13H26N4OS2Si/c1-14-12(19)15-9-7-6-8-10-11(18-21(3,4)5)17(2)13(20)16-10
InchiKey: RTZNTHYYTJDRKO-UHFFFAOYSA-N
Formula: C13H26N4OS2Si
SMILES: CNC(=S)NCCCCc1[nH]c(=S)n(C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 346.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	2.231		Crippen Method
rinpol	2326.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525367&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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<https://www.chemeo.com/cid/38-454-6/epsilon-Methylthiocarbamyl-lysine-MTH-TMS.pdf>

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