L-Cystathionine, N,N'-bis(tert-butyldimethylsilyl)-, bis(tert-butyldimethylsilyl) ester

Other names: L-cystathionine, 8tbdms derivative

Inchi: InChI=1S/C31H70N2O4SSi4/c1-28(2,3)39(13,14)32-24(26(34)36-41(17,18)30(7,8)9)21-2

InchiKey: SKJDCTIDDCKYEU-UHFFFAOYSA-N

Formula: C31H70N2O4SSi4

SMILES: CC(C)(C)[Si](C)(C)NC(CCSCC(N[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C)C(=O)O

Mol. weight [g/mol]: 679.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	9.133		Crippen Method
rinpol	3023.30		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333967&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices