N-Carbamyl-3-alanine, tris-TMS

Inchi: InChI=1S/C13H32N2O3Si3/c1-19(2,3)15-13(18-21(7,8)9)14-11-10-12(16)17-20(4,5)6/h1
InchiKey: UKUVFSKUBMPQNJ-UHFFFAOYSA-N
Formula: C13H32N2O3Si3
SMILES: C[Si](C)(C)NC(=NCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 348.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.29		Crippen Method
logp	3.387		Crippen Method
rinpol	1671.00		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=R401286&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices