N-Carbamyl-3-alanine, mono-TMS

Inchi: InChI=1S/C7H16N2O3Si/c1-13(2,3)12-6(10)4-5-9-7(8)11/h4-5H2,1-3H3,(H3,8,9,11)
InchiKey: TXQRASDZXHWBBY-UHFFFAOYSA-N
Formula: C7H16N2O3Si
SMILES: C[Si](C)(C)OC(=O)CCNC(N)=O
Mol. weight [g/mol]: 204.30

Physical Properties

Property code	Value	Unit	Source
log10ws	0.96		Crippen Method
logp	0.423		Crippen Method
rinpol	1209.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401271&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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