

N-Carbamyl-3-alanine, bis-TMS

Inchi: InChI=1S/C10H24N2O3Si2/c1-16(2,3)14-9(13)7-8-12-10(11)15-17(4,5)6/h7-8H2,1-6H3,(
InchiKey: SVQKQYXVQRXDQB-UHFFFAOYSA-N
Formula: C10H24N2O3Si2
SMILES: C[Si](C)(C)OC(=O)CCN=C(N)O[Si](C)(C)C
Mol. weight [g/mol]: 276.48

Physical Properties

Property code	Value	Unit	Source
log10ws	2.35		Crippen Method
logp	1.921		Crippen Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401266&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/123-149-0/N-Carbamyl-3-alanine-bis-TMS.pdf>

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