

Anserine, TMS

Inchi: InChI=1S/C16H32N4O3Si2/c1-20-12-17-11-13(20)10-14(16(22)23-25(5,6)7)19-15(21)8-9
InchiKey: YLCPMWYAQRTZKQ-UHFFFAOYSA-N
Formula: C16H32N4O3Si2
SMILES: Cn1cncc1CC(NC(=O)CCN[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 384.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	1.640		Crippen Method
rinpol	2598.00		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=R400703&Units=SI>

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/32-884-5/Anserine-TMS.pdf>

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