Pyrimidine, 6-amino-4-hydroxy-5-(3-carboxypropionyl)amino, TMS

InChI: InChI=1S/C17H34N4O4Si3/c1-26(2,3)21-16-15(17(19-12-18-16)25-28(7,8)9)20-13(22)10
InchiKey: YTDYLZKOUHTLGK-UHFFFAOYSA-N
Formula: C17H34N4O4Si3
SMILES: C[Si](C)(C)Nc1ncnc(O[Si](C)(C)C)c1NC(=O)CCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 442.73

Physical Properties

Property code	Value	Unit	Source
log10ws	1.88		Crippen Method
logp	4.034		Crippen Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		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=R387056&Units=SI

Legend

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