Pyroglutamic acid, MO TBDMS

Inchi: InChI=1S/C17H35NO3Si2/c1-16(2,3)22(7,8)20-14-12-11-13(18-14)15(19)21-23(9,10)17(
InchiKey: AYWIFAQPLFQPEW-UHFFFAOYSA-N
Formula: C17H35NO3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C1CCC(O[Si](C)(C)C(C)(C)C)=N1
Mol. weight [g/mol]: 357.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	5.117		Crippen Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		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=R564931&Units=SI

Legend

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