N-Acetylaspartylglutamic acid, tris(tert-butyldimethylsilyl) ester

Other names: (S)-Bis(tert-butyldimethylsilyl) 2-((S)-2-acetamido-4-[(tert-butyldimethylsilyl)oxy]-4-oxobutanamido)pentanedioate
(S)-Bis(tert-butyldimethylsilyl) 2-[(S)-2-acetamido-4-[(tert-butyldimethylsilyl)oxy]-4-oxobutanamido]pentanedioate

Inchi: InChI=1S/C29H58N2O8Si3/c1-20(32)30-22(19-24(34)38-41(13,14)28(5,6)7)25(35)31-21(

InchiKey: CBYJSCRGGDLHAO-UHFFFAOYSA-N

Formula: C29H58N2O8Si3

SMILES: CC(=O)NC(CC(=O)O[Si](C)(C)C(C)(C)C)C(=O)NC(CCC(=O)O[Si](C)(C)C(C)(C)C)C(=O)

Mol. weight [g/mol]: 647.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	5.791		Crippen Method
rinpol	3216.00		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=U378728&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices