N-Acetylaspartylglutamic acid, tris(trimethylsilyl) ester

Other names: (S)-Bis(trimethylsilyl) 2-((S)-2-acetamido-4-oxo-4-[(trimethylsilyl)oxy]butanamido)pentanedioate
(S)-Bis(trimethylsilyl) 2-[(S)-2-acetamido-4-oxo-4-[(trimethylsilyl)oxy]butanamido]pentanedioate

Inchi: InChI=1S/C20H40N2O8Si3/c1-14(23)21-16(13-18(25)29-32(5,6)7)19(26)22-15(20(27)30

InchiKey: AXTJSBBPEHHGTC-UHFFFAOYSA-N

Formula: C20H40N2O8Si3

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

Mol. weight [g/mol]: 520.80

Physical Properties

Property code	Value	Unit	Source
log10ws	2.87		Crippen Method
logp	3.961		Crippen Method
rinpol	2556.00		NIST Webbook
rinpol	2556.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U378754&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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