Homophenylalanine, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C19H31NO4Si/c1-7-23-18(22)20-16(14-13-15-11-9-8-10-12-15)17(21)24-25(5,

InchiKey: OXIBEQUOBLUWFK-UHFFFAOYSA-N

Formula: C19H31NO4Si

SMILES: CCOC(=O)NC(CCc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 365.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	4.282		Crippen Method
rinpol	2239.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R564431&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