Phe isoBOC TBDMS

Other names: Phe, N-isoBOC TBDMS
Inchi: InChI=1S/C20H33NO4Si/c1-15(2)14-24-19(23)21-17(13-16-11-9-8-10-12-16)18(22)25-26
InchiKey: YAVBGMXIEQOMRH-UHFFFAOYSA-N
Formula: C20H33NO4Si
SMILES: CC(C)COC(O)=NC(Cc1ccccc1)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 379.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	4.733		Crippen Method
rinpol	2254.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2254.00		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=R68900&Units=SI

Legend

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