Phenylalanine, MTH-TMS

Inchi: InChI=1S/C14H20N2OSSi/c1-16-13(17-19(2,3)4)12(15-14(16)18)10-11-8-6-5-7-9-11/h5-
InchiKey: XAGCENMTJPGXCP-UHFFFAOYSA-N
Formula: C14H20N2OSSi
SMILES: Cn1c(O[Si](C)(C)C)c(Cc2ccccc2)[nH]c1=S
Mol. weight [g/mol]: 292.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.405		Crippen Method
rinpol	2005.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525481&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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