Phenylalanine, mono-TMS

Inchi: InChI=1S/C12H19NO2Si/c1-16(2,3)13-11(12(14)15)9-10-7-5-4-6-8-10/h4-8,11,13H,9H2,
InchiKey: GGROBZMHJUTPPE-UHFFFAOYSA-N
Formula: C12H19NO2Si
SMILES: C[Si](C)(C)NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]: 237.37
CAS: 5269-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	2.107		Crippen Method
rinpol	1559.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1559.00		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=C5269443&Units=SI

Legend

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