

d5-phenylalanine, di-TMS

Inchi: InChI=1S/C15H27NO2Si2/c1-19(2,3)16-14(15(17)18-20(4,5)6)12-13-10-8-7-9-11-13/h7-14
InchiKey: DWNFNBPPSFIIBG-RAGZBHKVSA-N
Formula: C15H22D5NO2Si2
SMILES: C[Si](C)(C)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 314.58

Physical Properties

Property code	Value	Unit	Source
log10ws	0.53		Crippen Method
logp	3.400		Crippen Method
rinpol	1649.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R274856&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/28-916-4/d5-phenylalanine-di-TMS.pdf>

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