N-Acetyltyrosine, mono-TMS

Inchi: InChI=1S/C14H21NO4Si/c1-10(16)15-13(14(18)19-20(2,3)4)9-11-5-7-12(17)8-6-11/h5-8,
InchiKey: LOZDSIMIFWFOKE-UHFFFAOYSA-N
Formula: C14H21NO4Si
SMILES: CC(=O)NC(Cc1ccc(O)cc1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 295.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	1.817		Crippen Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R401251&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

Latest version available from:
https://www.chemeo.com/cid/117-424-1/N-Acetyltyrosine-mono-TMS.pdf
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