N-Acetyl-Try, TMS

Inchi: InChI=1S/C19H30N2O3Si2/c1-14(22)20-17(19(23)24-26(5,6)7)12-15-13-21(25(2,3)4)18-
InchiKey: CDCAQCWWNSIASG-UHFFFAOYSA-N
Formula: C19H30N2O3Si2
SMILES: CC(=O)NC(Cc1cn([Si](C)(C)C)c2ccccc12)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 390.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	3.750		Crippen Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		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=R95135&Units=SI

Legend

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