2-Pyrrolidino-1-(p-tolyl)-1-trimethylsilyloxyhexane

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M, (dihydro-), TMS
Inchi: InChI=1S/C20H35NOSi/c1-6-7-10-19(21-15-8-9-16-21)20(22-23(3,4)5)18-13-11-17(2)12-
InchiKey: KEECTUMXPMXXKJ-UHFFFAOYSA-N
Formula: C20H35NOSi
SMILES: CCCCC(C(O[Si](C)(C)C)c1ccc(C)cc1)N1CCCC1
Mol. weight [g/mol]: 333.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	5.542		Crippen Method
rinpol	1900.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1900.00		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=U314307&Units=SI

Legend

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