

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.cheméo.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

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