4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (HO-) TMS

Inchi: InChI=1S/C18H29NO2Si/c1-5-17(19-12-6-7-13-19)18(20)16-10-8-15(9-11-16)14-21-22(2

InchiKey: SJBFHEPMIDWQBM-UHFFFAOYSA-N

Formula: C18H29NO2Si

SMILES: CCC(C(=O)c1ccc(CO[Si](C)(C)C)cc1)N1CCCC1

Mol. weight [g/mol]: 319.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	4.095		Crippen Method
rinpol	2145.00		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=R417404&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices