Pyrrolidin-2-one, 1-[1-(4-trimethylsilyloxycarbonylphenyl)butan-1-o

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-oxo-) TMS
Inchi: InChI=1S/C18H25NO4Si/c1-5-15(19-12-6-7-16(19)20)17(21)13-8-10-14(11-9-13)18(22)2
InchiKey: OPWTYDXWQFENCU-UHFFFAOYSA-N
Formula: C18H25NO4Si
SMILES: CCC(C(=O)c1ccc(C(=O)O[Si](C)(C)C)cc1)N1CCCC1=O
Mol. weight [g/mol]: 347.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	3.262		Crippen Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360394&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