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

Other names: 4-methyl-«alpha»-pyrrolidinobutyrophenone-M (carboxy-oxo-dihydro-) diTMS

Inchi: InChI=1S/C21H35NO4Si2/c1-8-18(22-15-9-10-19(22)23)20(25-27(2,3)4)16-11-13-17(14-

InchiKey: NEDHARLTVIMVAU-UHFFFAOYSA-N

Formula: C21H35NO4Si2

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

Mol. weight [g/mol]: 421.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	4.972		Crippen Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360395&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices