Benzoic acid, 4-(1-trimethylsilyloxy)-2-(pyrrolidin-1-yl)butyl-, trimethylsilyl ester

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

Inchi: InChI=1S/C21H37NO3Si2/c1-8-19(22-15-9-10-16-22)20(24-26(2,3)4)17-11-13-18(14-12-

InchiKey: GHSNXQLJVMPZLH-UHFFFAOYSA-N

Formula: C21H37NO3Si2

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

Mol. weight [g/mol]: 407.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	5.445		Crippen Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		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=U360391&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices