R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone (carboxy-HO-alkyl-), 2TMS

Inchi: InChI=1S/C23H39NO4Si2/c1-8-11-20(27-29(2,3)4)21(24-16-9-10-17-24)22(25)18-12-14-

InchiKey: LIXHUYQNESGUCK-UHFFFAOYSA-N

Formula: C23H39NO4Si2

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

Mol. weight [g/mol]: 449.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	5.346		Crippen Method
rinpol	2625.00		NIST Webbook
rinpol	2635.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290794&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