«alpha»-Aminopimelic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C22H45NO6Si2/c1-12-27-20(26)23-17(19(25)29-31(10,11)22(5,6)7)15-13-14-1

InchiKey: XNTQTIDDZFSXLY-UHFFFAOYSA-N

Formula: C22H45NO6Si2

SMILES: CCOC(=O)NC(CCCCC(=O)O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 475.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	5.758		Crippen Method
rinpol	2510.00		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=R562693&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices