Trimethylsilyl 4-bis(trimethylsilyloxy)phosphorylbutanoate

Inchi: InChI=1S/C13H33O5PSi3/c1-20(2,3)16-13(14)11-10-12-19(15,17-21(4,5)6)18-22(7,8)9/h

InchiKey: XQFRLDBVUGLFBI-UHFFFAOYSA-N

Formula: C13H33O5PSi3

SMILES: C[Si](C)(C)OC(=O)CCCP(=O)(O[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 384.63

Physical Properties

Property code	Value	Unit	Source
log10ws	1.27		Crippen Method
logp	5.041		Crippen Method
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U372925&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