tert-Butyldimethylsilyl 2-bis(tert-butyldimethylsilyloxy)phosphorylbutano

Other names: 2-Phosphonobutanoic acid, tris-tert-butyldimethylsilyl

Inchi: InChI=1S/C22H51O5PSi3/c1-17-18(19(23)25-29(11,12)20(2,3)4)28(24,26-30(13,14)21(5

InchiKey: YUUMOIPQRNNCMM-UHFFFAOYSA-N

Formula: C22H51O5PSi3

SMILES: CCC(C(=O)O[Si](C)(C)C(C)(C)C)P(=O)(O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 510.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	8.550		Crippen Method
rinpol	2149.00		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=U378228&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices