

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

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/ci9903071
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

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