

tert-Butyldimethylsilyl 4-bis(tert-butyldimethylsilyloxy)phosphorylbutanoate

Other names:	4-Phosphonobutanoic acid, tris-tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C22H51O5PSi3/c1-20(2,3)29(10,11)25-19(23)17-16-18-28(24,26-30(12,13)21(14,15)22)/p1
InchiKey:	FXIHEDPQRNNRHL-UHFFFAOYSA-N
Formula:	C22H51O5PSi3
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CCCP(=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	-2.50		Crippen Method
logp	8.552		Crippen Method
rinpol	2381.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373097&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

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