

4-Bis[(tert-butyl dimethylsilyl)oxy]phosphoryl-N-(tert-butyl)butylphosphonate

Other names:	Bis(tert-butyl dimethylsilyl) 4-[(tert-butyl dimethylsilyl)amino]butylphosphonate Phosphonic acid, [4-[(tert-butyl dimethylsilyl)amino]butyl]-, bis(tert-butyl dimethylsilyl) ester
Inchi:	InChI=1S/C22H54NO3PSi3/c1-20(2,3)28(10,11)23-18-16-17-19-27(24,25-29(12,13)21(4
InchiKey:	VJADKNFWFEYJP-UHFFFAOYSA-N
Formula:	C22H54NO3PSi3
SMILES:	CC(C)(C)[Si](C)(C)NCCCCP(=O)(O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	495.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	8.598		Crippen Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/59-648-8/4-Bis-tert-butyl dimethylsilyl-oxy-phosphoryl-N-tert-butyl dimethylsilyl-butan-1-ylphosphonate>

Generated by Cheméo on 2024-05-01 02:01:10.780434207 +0000 UTC m=+16818119.701011517.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.