

Bis(trimethylsilyl) 4-[bis(trimethylsilyl)amino]butylphosphonate

Other names:

Phosphonic acid, [4-[bis(trimethylsilyl)amino]butyl]-, bis(trimethylsilyl) ester

4-Bis(trimethylsilyloxy)phosphoryl-N,N-bis(trimethylsilyl)butan-1-amine

Inchi:

InChI=1S/C16H44NO3PSi4/c1-22(2,3)17(23(4,5)6)15-13-14-16-21(18,19-24(7,8)9)20-25

InchiKey:

NKHPRDOLUKUGPH-UHFFFAOYSA-N

Formula:

C16H44NO3PSi4

SMILES:

C[Si](C)(C)OP(=O)(CCCCN([Si](C)(C)C)[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]:

441.84

Physical Properties

Property code	Value	Unit	Source
log10ws	2.26		Crippen Method
logp	6.634		Crippen Method
rinpol	1983.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U373035&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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.chemeo.com/cid/39-875-8/Bis-trimethylsilyl-4-bis-trimethylsilyl-amino-butylphosphonate.pdf>

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