Bialophos, N,O,O-tris(tert-butyldimethylsilyl)deriv.

Other names: Bialaphos, TBDMS

Inchi: InChI=1S/C29H64N3O6PSi3/c1-21(24(33)31-22(2)26(35)37-41(15,16)28(6,7)8)30-25(34

InchiKey: GZDXBWHGVVXWAA-UHFFFAOYSA-N

Formula: C29H64N3O6PSi3

SMILES: CC(NC(=O)C(CCP(C)(=O)O[Si](C)(C)C(C)(C)C)N[Si](C)(C)C(C)(C)C)C(=O)NC(C)C(=O)

Mol. weight [g/mol]: 666.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	6.827		Crippen Method

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=U292763&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient