Heptanedioic acid, bis(tert-butyldimethylsilyl) ester

Other names: Pimelic acid, bis(tert-butyldimethylsilyl) ester
Pimelic acid, diTBDMS
Pimelic acid, DMTBS
Pimelic acid, TBDMS
Bis[tert-butyl(dimethyl)silyl] pimelate
Heptanedioic acid, 2tbdms derivative

Inchi: InChI=1S/C19H40O4Si2/c1-18(2,3)24(7,8)22-16(20)14-12-11-13-15-17(21)23-25(9,10)19

InchiKey: BBMNMSUSTQGVGW-UHFFFAOYSA-N

Formula: C19H40O4Si2

SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCCCCC(=O)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 388.69

CAS: 104255-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	6.034		Crippen Method
rinpol	2071.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2066.00		NIST Webbook
rinpol	2059.80		NIST Webbook
rinpol	2059.80		NIST Webbook

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=C104255950&Units=SI

Legend

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