Pentanedioic acid, 3-methyl-, bis(tert-butyldimethylsilyl) ester

Other names: 3-Methylglutaric acid, diTBDMS
3-Methylglutaric acid, DMTBS
3-Methylglutaric acid, TBDMS
3-Methylpentanedioic acid, 2tbdms derivative

Inchi: InChI=1S/C18H38O4Si2/c1-14(12-15(19)21-23(8,9)17(2,3)4)13-16(20)22-24(10,11)18(5,

InchiKey: IUTZKFAHABEWKJ-UHFFFAOYSA-N

Formula: C18H38O4Si2

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

Mol. weight [g/mol]: 374.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	5.499		Crippen Method
rinpol	1873.00		NIST Webbook
rinpol	1870.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1873.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U221766&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