

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, 2tbds 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/ci990307I

Legend

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

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