

Butanedioic acid, methyl-, bis(tert-butyldimethylsilyl) ester

Other names:

Methylsuccinic acid, bis-TBDMS
Methylsuccinic acid, bis(tert-butyldimethylsilyl) ester
Methylsuccinic acid, diTBDMS
Methylsuccinic acid, bis-TBDMS ester
Methylsuccinic acid, TBDMS
Methylsuccinic acid, DMTBS
Bis[tert-butyl(dimethyl)silyl] 2-methylsuccinate
Methylsuccinic acid, 2tbds derivative

Inchi:

InChI=1S/C17H36O4Si2/c1-13(15(19)21-23(10,11)17(5,6)7)12-14(18)20-22(8,9)16(2,3)4

InchiKey:

RMDDLEXHNWAQGQ-UHFFFAOYSA-N

Formula:

C17H36O4Si2

SMILES:

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

Mol. weight [g/mol]:

360.64

CAS:

98830-33-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.52		Crippen Method
logp	5.109		Crippen Method
rinpol	1770.00		NIST Webbook
rinpol	1759.10		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1759.10		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=C98830332&Units=SI>

Legend

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

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