

Pentanedioic acid, bis(tert-butyldimethylsilyl) ester

Other names:

Glutaric acid, bis-TBDMS
Glutaric acid, bis(tert-butyldimethylsilyl) ester
Glutaric acid, diTBDMS
Glutaric acid, bis-TBDMS ester
Glutaric acid, TBDMS
Glutarate, TBDMS
Glutaric acid, DMTBS
Pentanedioic acid, 2tbdms derivative

Inchi:

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

InchiKey:

CGCYGKFYZGUDQP-UHFFFAOYSA-N

Formula:

C17H36O4Si2

SMILES:

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

Mol. weight [g/mol]:

360.64

CAS:

98830-34-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.77		Crippen Method
logp	5.253		Crippen Method
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1851.20		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1855.12		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1851.20		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C98830343&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Legend

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

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