Propanedioic acid, dimethyl-, bis(tert-butyldimethylsilyl) ester

Other names: Dimethylmalonic acid, TBDMS
Inchi: InChI=1S/C17H36O4Si2/c1-15(2,3)22(9,10)20-13(18)17(7,8)14(19)21-23(11,12)16(4,5)6
InchiKey: ZBYZHGVYKOKRAB-UHFFFAOYSA-N
Formula: C17H36O4Si2
SMILES: CC(C)(C(=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: 98830-31-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.52		Crippen Method
logp	5.109		Crippen Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98830310&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