Butanedioic acid, 2-[(tert-butyldimethylsilyl)oxy]-, bis(tert-butyldimethylsilyl) ester

Other names: DL-Malic acid, 2-tert-butyldimethylsilyl-, bis(tert-butyldimethylsilyl) ester
Malic acid, tris-TBDMS
Malic acid, TBDMS
Malic acid, DMTBS
Malic acid, 3tbdms derivative

Inchi: InChI=1S/C22H48O5Si3/c1-20(2,3)28(10,11)25-17(19(24)27-30(14,15)22(7,8)9)16-18(23

InchiKey: LGKDLSNIOMYKSN-UHFFFAOYSA-N

Formula: C22H48O5Si3

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

Mol. weight [g/mol]: 476.87

CAS: 99461-86-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.11		Crippen Method
logp	6.864		Crippen Method
rinpol	2115.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2094.50		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=C99461866&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices