Tris(dimethyl-t-butylsilyl) O-(dimethyl-t-butylsilyl)citrate

Other names: 1,2,3-Propanetricarboxylic acid, 2-[(tert-butyldimethylsilyl)oxy]-, tris(tert-butyldimethylsilyl) ester
Citric acid, (4TBDMS)-
Citric acid, tetraTBDMS
Citric acid, TBDMS
Citric acid, 4tbdms derivative

Inchi: InChI=1S/C30H64O7Si4/c1-26(2,3)38(13,14)34-23(31)21-30(37-41(19,20)29(10,11)12,25

InchiKey: LYMHMSBQXFZXLH-UHFFFAOYSA-N

Formula: C30H64O7Si4

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

Mol. weight [g/mol]: 649.17

CAS: 99477-48-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.37		Crippen Method
logp	9.172		Crippen Method
rinpol	2622.00		NIST Webbook
rinpol	2589.60		NIST Webbook
rinpol	2617.00		NIST Webbook
rinpol	2622.00		NIST Webbook
rinpol	2625.00		NIST Webbook
rinpol	2589.60		NIST Webbook
rinpol	2625.00		NIST Webbook
rinpol	2626.00		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=C99477482&Units=SI

Legend

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