Pentaric acid, 2,3-dideoxy-4-O-(trimethylsilyl)-3-[[(trimethylsilyl)oxy]bis(trimethylsilyl) ester

Other names:	1,2,3-Propanetricarboxylic acid, 1-[(trimethylsilyl)oxy]-, tris(trimethylsilyl) ester
	tris(Trimethylsilyl) isocitrate, (trimethylsilyl)oxy-
	Isocitric acid (4TMS)
	Isocitric acid, tetrakis-TMS
	Isocitric acid, tetra-TMS
	Propane-1,2,3-tricarboxylic acid, 1-hydroxy, tetrakis-TMS
	Isocitric acid, TMS
Inchi:	InChI=1S/C18H40O7Si4/c1-26(2,3)22-15(19)13-14(17(20)24-28(7,8)9)16(23-27(4,5)6)18
InchiKey:	QMCRZQSRNUSJRR-UHFFFAOYSA-N
Formula:	C18H40O7Si4
SMILES:	C[Si](C)(C)OC(=O)CC(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	480.85
CAS:	55517-57-2

Physical Properties

Property code	Value	Unit	Source
log10ws	4.89		Crippen Method
logp	4.347		Crippen Method
rinpol	1841.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1818.80		NIST Webbook
rinpol	1851.00		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=C55517572&Units=SI

Legend

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