

Methylcitric acid, tetra-TMS, #1

Other names:	Methylcitric acid, tetraTMS (1)
Inchi:	InChI=1S/C19H42O7Si4/c1-15(17(21)24-28(5,6)7)19(26-30(11,12)13,18(22)25-29(8,9)10
InchiKey:	HPVCSLKJFDTUAG-UHFFFAOYSA-N
Formula:	C19H42O7Si4
SMILES:	CC(C(=O)O[Si](C)(C)C)C(CC(=O)O[Si](C)(C)C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	494.87

Physical Properties

Property code	Value	Unit	Source
log10ws	4.48		Crippen Method
logp	4.737		Crippen Method
rinpola	1862.00		NIST Webbook
rinpola	1961.00		NIST Webbook
rinpola	1862.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R51866&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/122-842-1/Methylcitric-acid-tetra-TMS-1.pdf>

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