

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

Other names:

1,2,3-Propanetricarboxylic acid, 2-[(tert-butyl dimethylsilyl)oxy]-,  
tris(tert-butyl dimethylsilyl) 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)12,2,

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	2626.00		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

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C99477482&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

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

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