

1,2,3-Propanetricarboxylic acid, 2-[(trimethylsilyl)oxy]-, tris(trimethylsilyl)

Other names:
ester

Citric acid, tetrakis(trimethylsilyl) deriv.

Tris(trimethylsilyl) 2-[(trimethylsilyl)oxy]-1,2,3-propanetricarboxylate

Citric acid, tetrakis-TMS

Citric acid, tetra-TMS

Citric acid, TMS

Citric acid, trimethylsilyl ether, tris(trimethylsilyl) ester

Citric acid, (4TMS)

Propane-1,2,3-tricarboxylic acid, 2-trimethylsilyloxy, tris-trimethylsilyl ester

Citric acid, 4tms derivative

Inchi: InChI=1S/C18H40O7Si4/c1-26(2,3)22-15(19)13-18(25-29(10,11)12,17(21)24-28(7,8)9)14

InchiKey: VFGAVMGYDWDESE-UHFFFAOYSA-N

Formula: C18H40O7Si4

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

Mol. weight [g/mol]: 480.85

CAS: 14330-97-3

Physical Properties

Property code	Value	Unit	Source
log10ws	4.65		Crippen Method
logp	4.491		Crippen Method
rinpol	1815.70		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1815.70		NIST Webbook

rropol	1839.00	NIST Webbook
rropol	1800.00	NIST Webbook
rropol	1857.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C14330973&Units=SI>

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

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rropol: Non-polar retention indices

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