

Pentanedioic acid, 3-methyl-3-[(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester

Other names: «beta»-Hydroxy-«beta»-methylglutaric acid (3TMS)
3-Trimethylsilyloxy-3-methyl-bis(trimethylsilyl)glutarate

3-Hydroxy-3-methylglutaric acid, tris(trimethylsilyl) deriv.

3-Hydroxy-3-methylglutaric acid, tri-TMS

Glutaric acid, 3-hydroxy-3-methyl, tris-TMS

3-Hydroxy-3-methylglutaric acid, TMS # 2

«beta»-Hydroxy-«beta»-methylglutaric acid (tms)

3-Hydroxy-3-methylglutarate, TMS

2,4-Dideoxy-3-C-methylpentaric acid, TMS

3-Hydroxy-3-methylglutaric acid, TMS

Inchi: InChI=1S/C15H34O5Si3/c1-15(20-23(8,9)10,11-13(16)18-21(2,3)4)12-14(17)19-22(5,6)7

InchiKey: SWDDFRVEZJUJJD-UHFFFAOYSA-N

Formula: C15H34O5Si3

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

Mol. weight [g/mol]: 378.68

CAS: 55590-95-9

Physical Properties

Property code	Value	Unit	Source
log10ws	2.82		Crippen Method
logp	4.133		Crippen Method
rinpol	1612.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1582.70		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1647.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55590959&Units=SI>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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