

Pentanedioic acid, 3-methyl-, bis(trimethylsilyl) ester

Other names:	3-Methylglutaric acid, bis(trimethylsilyl)-, ester 3-Methylglutaric acid, di(trimethylsilyl) ester 3-Methylglutaric acid, bis(trimethylsilyl ester) 3-Methylglutaric acid, diTMS 3-Methylglutaric acid, bis-TMS ester Glutaric acid, 3-methyl, bis-TMS 3-Methylglutaric acid, TMS 3-Methylglutaric acid, 2tms derivative
Inchi:	InChI=1S/C12H26O4Si2/c1-10(8-11(13)15-17(2,3)4)9-12(14)16-18(5,6)7/h10H,8-9H2,1-7H3
InchiKey:	JOPZTTHKNFWHFT-UHFFFAOYSA-N
Formula:	C12H26O4Si2
SMILES:	CC(CC(=O)O[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	290.50
CAS:	55517-41-4

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	3.159		Crippen Method
rinpol	1431.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1431.00		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=C55517414&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/59-346-3/Pentanedioic-acid-3-methyl-bis-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-05 15:36:24.543655242 +0000 UTC m=+17212633.464232557.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.