

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

Other names:

3-Methyladipic acid (2TMS)
3-Methyladipic acid, bis(trimethylsilyl)-, ester
3-Methyladipic acid, diTMS
Hexanedioic acid, 3-methyl-, 1,6-bis(trimethylsilyl) ester
3-Methyladipic acid (tms)
3-Methyladipic acid, 2tms derivative

Inchi: InChI=1S/C13H28O4Si2/c1-11(10-13(15)17-19(5,6)7)8-9-12(14)16-18(2,3)4/h11H,8-10H

InchiKey: IDHDZCKJOKHATB-UHFFFAOYSA-N

Formula: C13H28O4Si2

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

Mol. weight [g/mol]: 304.53

CAS: 55520-93-9

Physical Properties

Property code	Value	Unit	Source
log10ws	1.15		Crippen Method
logp	3.549		Crippen Method
rinpol	1528.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1522.90		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1522.90		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1539.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C55520939&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

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.cheméo.com/cid/124-343-3/Hexanedioic-acid-3-methyl-bis-trimethylsilyl-ester.pdf>

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