

Pentanedioic acid, 2-methyl-, bis(trimethylsilyl) ester

Other names: 2-Methylglutaric acid, bis(trimethylsilyl)- ester

2-Methylglutaric acid, 2tms derivative

Inchi: InChI=1S/C12H26O4Si2/c1-10(12(14)16-18(5,6)7)8-9-11(13)15-17(2,3)4/h10H,8-9H2,1-7

InchiKey: GRKPITUYBIOOJQ-UHFFFAOYSA-N

Formula: C12H26O4Si2

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

Mol. weight [g/mol]: 290.50

CAS: 55530-53-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.57		Crippen Method
logp	3.159		Crippen Method
rinpol	1407.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1423.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55530535&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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