

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

Other names:	3,3-Dimethylglutaric acid, bis-TMS 3,3-dimethylglutaric acid, TMS 3,3-Dimethylglutaric acid, 2tms derivative
Inchi:	InChI=1S/C13H28O4Si2/c1-13(2,9-11(14)16-18(3,4)5)10-12(15)17-19(6,7)8/h9-10H2,1-8
InchiKey:	BOQKCPUOQCUQAI-UHFFFAOYSA-N
Formula:	C13H28O4Si2
SMILES:	CC(C)(CC(=O)O[Si](C)(C)C)CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	304.53
CAS:	55887-57-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.15		Crippen Method
logp	3.549		Crippen Method
rinpol	1431.00		NIST Webbook
rinpol	1431.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55887575&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/14-841-2/Pentanedioic-acid-3-3-dimethyl-bis-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-05-02 16:39:38.446069825 +0000 UTC m=+16957227.366647141.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.