

3-Methylglutaconic acid, diTMS

Inchi: InChI=1S/C13H26O3Si2/c1-11(9-12(2)15-17(3,4)5)10-13(14)16-18(6,7)8/h10H,2,9H2,1,3
InchiKey: UDLFOGZQPIYHEL-ZHACJKMWSA-N
Formula: C13H26O3Si2
SMILES: C=C(CC(C)=CC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 286.51

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	4.066		Crippen Method
rinpol	1417.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1417.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273086&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/123-923-0/3-Methylglutaconic-acid-diTMS.pdf>

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