

C-Methylglyceraric acid, TMS

Inchi: InChI=1S/C13H30O5Si3/c1-13(18-21(8,9)10,11(14)16-19(2,3)4)12(15)17-20(5,6)7/h1-10
InchiKey: JGZMZMIPCIWFLE-UHFFFAOYSA-N
Formula: C13H30O5Si3
SMILES: CC(O[Si](C)(C)C)(C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 350.63

Physical Properties

Property code	Value	Unit	Source
log10ws	3.66		Crippen Method
logp	3.353		Crippen Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R101674&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

Latest version available from:

<https://www.chemeo.com/cid/117-310-7/C-Methylglyceraric-acid-TMS.pdf>

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