C-Methylthrearic acid, TMS

Inchi: InChI=1S/C17H40O6Si4/c1-17(23-27(11,12)13,16(19)22-26(8,9)10)14(20-24(2,3)4)15(18
InchiKey: JCFLZSFDCXYOFI-PBHICJAKSA-N
Formula: C17H40O6Si4
SMILES: CC(O[Si](C)(C)C)(C(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 452.84

Physical Properties

Property code	Value	Unit	Source
log10ws	4.73		Crippen Method
logp	4.573		Crippen Method
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R101689&Units=SI

Legend

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