METHYLCITRIC ACID (II) diTMS

Inchi: InChI=1S/C16H34O6Si3/c1-12(15(18)21-24(5,6)7)13(16(19)22-25(8,9)10)11-14(17)20-23
InchiKey: ZIBWAZOBHCXEOD-UHFFFAOYSA-N
Formula: C16H34O6Si3
SMILES: CC(C(=O)O[Si](C)(C)C)C(CC(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 406.69

Physical Properties

Property code	Value	Unit	Source
log10ws	3.22		Crippen Method
logp	3.763		Crippen Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		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=R395963&Units=SI

Legend

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