Methylcitric acid, TBDMS # 1

Inchi: InChI=1S/C26H54O6Si3/c1-19(23(29)32-35(15,16)26(8,9)10)20(17-21(27)30-33(11,12)2
InchiKey: FIIBTZKDSXQOEQ-UHFFFAOYSA-N
Formula: C26H54O6Si3
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)C(CC(=O)O[Si](C)(C)C(C)(C)C)CC(=O)O[Si](C)(C)C(C)(C
Mol. weight [g/mol]: 546.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.96		Crippen Method
logp	7.664		Crippen Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		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=R564619&Units=SI

Legend

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