Ketopimelic acid, DMTBS

Inchi: InChI=1S/C25H52O5Si3/c1-23(2,3)31(10,11)28-20(22(27)30-33(14,15)25(7,8)9)18-16-17
InchiKey: KHPINZXMIAGANO-ZZEZOPTASA-N
Formula: C25H52O5Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCCC=C(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 516.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	8.159		Crippen Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R538333&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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