Benzylmalic acid, TBDMS

Inchi: InChI=1S/C29H54O5Si3/c1-27(2,3)35(10,11)32-24(26(31)34-37(14,15)29(7,8)9)23(21-22
InchiKey: SERKHULUKJGTSC-UHFFFAOYSA-N
Formula: C29H54O5Si3
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C(Cc1ccccc1)C(O[Si](C)(C)C(C)(C)C)C(=O)O[Si](C)(C)C(C)(C
Mol. weight [g/mol]: 566.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.332		Crippen Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R564000&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