Benzoic acid, 2-hydroxy, 3-(2,3-dioxypropyl), bis-DTBS

Inchi: InChI=1S/C26H44O5Si2/c1-23(2,3)32(24(4,5)6)28-17-19(29-32)16-18-14-13-15-20-21(18

InchiKey: TVWNOCFXIYYQPX-UHFFFAOYSA-N

Formula: C26H44O5Si2

SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC(=O)c2cccc(CC3CO[Si](C(C)(C)C)(C(C)(C)C)O3)c2O1

Mol. weight [g/mol]: 492.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	7.278		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41132&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