Benzene-1,4-dicarboxylic acid, 2,5-dihydroxy, bis-DTBS

Inchi: InChI=1S/C24H38O6Si2/c1-21(2,3)31(22(4,5)6)27-17-13-16-18(14-15(17)19(25)29-31)28

InchiKey: RBINJDPNHNBCHF-UHFFFAOYSA-N

Formula: C24H38O6Si2

SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC(=O)c2cc3c(cc2O1)C(=O)O[Si](C(C)(C)C)(C(C)(C)C)O3

Mol. weight [g/mol]: 478.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	6.870		Crippen Method
rinpol	2730.00		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=R41075&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices