Benzofuran-5-propanol, 2,3-dihydro-7-hydroxy-3-hydroxymethyl-2-(4-hydr tetrakis-TMS

Inchi: InChI=1S/C31H54O6Si4/c1-32-28-21-24(16-17-27(28)36-40(8,9)10)30-26(22-34-39(5,6)

InchiKey: ZBUBYKOLTNGICP-UHFFFAOYSA-N

Formula: C31H54O6Si4

SMILES: COc1cc(C2Oc3c(O[Si](C)(C)C)cc(CCCO[Si](C)(C)C)cc3C2CO[Si](C)(C)C)ccc1O[Si](C)(C

Mol. weight [g/mol]: 635.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.47		Crippen Method
logp	8.976		Crippen Method
rinpol	3027.00		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=R499500&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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