

Benzofuran-5-propanol, 2,3-dihydro-7-hydroxy-3-hydroxymethyl-2-(4-hydroxyphenyl)- tetraakis-TMS

InChI: CC1=CS/C31H54O6Si4/c1-32-28-21-24(16-17-27(28)36-40(8,9)10)30-26(22-34-39(5,6)40)1-2
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)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: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499500&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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