

Benzenepropanol, 3-hydroxy-4-(1-hydroxymethyl-2-(4-hydroxy-3-methoxyphenyl)propan-2-yl)phenyl tetraakis-TMS

InChI: InChI=1S/C31H56O5Si4/c1-32-31-23-26(17-19-29(31)35-39(8,9)10)21-27(24-34-38(5,6)39-40)41-42

InChIKey: QZBCJZUYLQPEQW-UHFFFAOYSA-N

Formula: C₃₁H₅₆O₅Si₄

SMILES: COc1cc(CC(CO[Si](C)(C)C)c2ccc(CCCO[Si](C)(C)C)cc2O[Si](C)(C)C)ccc1O[Si](C)(C)C

Mol. weight [g/mol]: 621.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	9.085		Crippen Method
rinpol	2982.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499466&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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<https://www.chemeo.com/cid/17-953-5/Benzenepropanol-3-hydroxy-4-1-hydroxymethyl-2-4-hydroxy-3-methoxyphenyl>

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