

Propanoic acid, 2-hydroxy-2-methyl-3-(4-hydroxy-3-methoxyphenyl)- tris-TMS

InChI: InChI=1S/C20H38O5Si3/c1-20(25-28(9,10)11,19(21)24-27(6,7)8)15-16-12-13-17(18(14-
InChIKey: RUODZGNCMAHFIP-UHFFFAOYSA-N
Formula: C20H38O5Si3
SMILES: COc1cc(CC(C)(O[Si](C)(C)C)C(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 442.77

Physical Properties

Property code	Value	Unit	Source
log10ws	1.09		Crippen Method
logp	5.440		Crippen Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R100577&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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