

1-Propanol, 3-(3,4-dihydroxyphenyl), tris-TMS

Inchi: InChI=1S/C18H36O3Si3/c1-22(2,3)19-14-10-11-16-12-13-17(20-23(4,5)6)18(15-16)21-22
InchiKey: WOMAGNBHYHREPP-UHFFFAOYSA-N
Formula: C18H36O3Si3
SMILES: C[Si](C)(C)OCCc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 384.73

Physical Properties

Property code	Value	Unit	Source
log10ws	0.90		Crippen Method
logp	5.898		Crippen Method
rinpol	1876.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R99866&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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<https://www.cheméo.com/cid/44-420-6/1-Propanol-3-3-4-dihydroxyphenyl-tris-TMS.pdf>

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