1,3,5-tris-(Hydroxymethyl) benzene, tris-TMS

Inchi: InChI=1S/C18H36O3Si3/c1-22(2,3)19-13-16-10-17(14-20-23(4,5)6)12-18(11-16)15-21-24
InchiKey: PDGOOYABJKELRY-UHFFFAOYSA-N
Formula: C18H36O3Si3
SMILES: C[Si](C)(C)OCc1cc(CO[Si](C)(C)C)cc(CO[Si](C)(C)C)c1
Mol. weight [g/mol]: 384.73

Physical Properties

Property code	Value	Unit	Source
log10ws	0.71		Crippen Method
logp	5.741		Crippen Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		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=R96351&Units=SI

Legend

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