4-tert-Butylcatechol, bis(tert-butyldimethylsilyl) ether

Other names: 4-Tert-butylcatechol, 2tbdms derivative
Inchi: InChI=1S/C22H42O2Si2/c1-20(2,3)17-14-15-18(23-25(10,11)21(4,5)6)19(16-17)24-26(12
InchiKey: XFAJEKRYVFCVMC-UHFFFAOYSA-N
Formula: C22H42O2Si2
SMILES: CC(C)(C)c1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 394.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	7.752		Crippen Method
rinpol	1983.10		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352798&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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