Anthracene, 1,2,3,4,5,6,7,8-octahydro-cis-1,2-diol, DTBS

Inchi: InChI=1S/C22H34O2Si/c1-21(2,3)25(22(4,5)6)23-19-12-11-17-13-15-9-7-8-10-16(15)14-

InchiKey: HRAYGHPOCVKHDZ-UXHICEINSA-N

Formula: C22H34O2Si

SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2CCc3cc4c(cc3C2O1)CCCC4

Mol. weight [g/mol]: 358.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	6.011		Crippen Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R115292&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