Phenanthrene, 9,10-dihydro-trans-9,10-diol, DTBS

Inchi: InChI=1S/C22H28O2Si/c1-21(2,3)25(22(4,5)6)23-19-17-13-9-7-11-15(17)16-12-8-10-14-

InchiKey: WEEBMLUMSOLDIX-PMACEKPBSA-N

Formula: C22H28O2Si

SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2c3ccccc3-c3ccccc3C2O1

Mol. weight [g/mol]: 352.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.71		Crippen Method
logp	6.539		Crippen Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		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=R115485&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices