

Phenanthrene, 9,10-dihydro-cis-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-BGYRXZFFSA-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	2360.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115470&Units=SI

Legend

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

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