

Anthracene, 1,2,3,4-tetrahydro-cis-1,2-diol, DTBS

Inchi:	InChI=1S/C22H30O2Si/c1-21(2,3)25(22(4,5)6)23-19-12-11-17-13-15-9-7-8-10-16(15)14-
InchiKey:	DGGGQPBNYLDKJF-UXHICEINSA-N
Formula:	C22H30O2Si
SMILES:	CC(C)(C)[Si]1(C(C)(C)C)OC2CCc3cc4ccccc4cc3C2O1
Mol. weight [g/mol]:	354.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	6.285		Crippen Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115301&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/45-193-8/Anthracene-1-2-3-4-tetrahydro-cis-1-2-diol-DTBS.pdf>

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