

Anthracene, 1,2-dihydro-trans-1,2-diol, DTBS

Inchi: InChI=1S/C22H28O2Si/c1-21(2,3)25(22(4,5)6)23-19-12-11-17-13-15-9-7-8-10-16(15)14-
InchiKey: OBXCROHLJUAMTP-WOJBJXKFSA-N
Formula: C22H28O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2C=Cc3cc4ccccc4cc3C2O1
Mol. weight [g/mol]: 352.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	6.365		Crippen Method
rinsol	2500.00		NIST Webbook
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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=R115321&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/22-713-5/Anthracene-1-2-dihydro-trans-1-2-diol-DTBS.pdf>

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