1,2-Naphthalenediol, DTBS

Inchi: InChI=1S/C18H24O2Si/c1-17(2,3)21(18(4,5)6)19-15-12-11-13-9-7-8-10-14(13)16(15)20-

InchiKey: RWZDPIAPAAPESQ-UHFFFAOYSA-N

Formula: C18H24O2Si

SMILES: CC(C)(C)[Si]1(C(C)(C)C)Oc2ccc3ccccc3c2O1

Mol. weight [g/mol]: 300.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	5.653		Crippen Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		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=R115232&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices