

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

Latest version available from:

<https://www.chemeo.com/cid/16-188-6/1-2-Naphthalenediol-DTBS.pdf>

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