

trans-2,3-Tetralinediol, DTBS

Inchi: InChI=1S/C18H28O2Si/c1-17(2,3)21(18(4,5)6)19-15-11-13-9-7-8-10-14(13)12-16(15)20-
InchiKey: ZGGDUGVGAUHMTA-HOTGVXAUSA-N
Formula: C18H28O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2Cc3ccccc3CC2O1
Mol. weight [g/mol]: 304.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	4.612		Crippen Method
rinpol	1960.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R115514&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/56-379-0/trans-2-3-Tetralinediol-DTBS.pdf>

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