

2,3,5-Tetralinetriol, DTBS, 5-TMS

Inchi: InChI=1S/C21H36O3Si2/c1-20(2,3)26(21(4,5)6)23-18-13-15-11-10-12-17(22-25(7,8)9)16
InchiKey: LKNCQPBOKVDBFA-UHFFFAOYSA-N
Formula: C21H36O3Si2
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2Cc3cccc(O[Si](C)(C)C)c3CC2O1
Mol. weight [g/mol]: 392.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	5.825		Crippen Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		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=R115267&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/37-520-3/2-3-5-Tetralinetriol-DTBS-5-TMS.pdf>

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