

2,3,5-Tetralinetriol, DTBS

Inchi: InChI=1S/C18H28O3Si/c1-17(2,3)22(18(4,5)6)20-15-10-12-8-7-9-14(19)13(12)11-16(15)
InchiKey: STDRGROWMFMIQN-UHFFFAOYSA-N
Formula: C18H28O3Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OC2Cc3cccc(O)c3CC2O1
Mol. weight [g/mol]: 320.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	4.317		Crippen Method
rinpol	2200.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R115252&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/81-984-0/2-3-5-Tetralinetriol-DTBS.pdf>

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