

Ethanediol, 1-phenyl, DTBS

Inchi: InChI=1S/C16H26O2Si/c1-15(2,3)19(16(4,5)6)17-12-14(18-19)13-10-8-7-9-11-13/h7-11,
InchiKey: VUPZMOJAPXXSPB-AWEZLNQCLSA-N
Formula: C16H26O2Si
SMILES: CC(C)(C)[Si]1(C(C)(C)C)OCC(c2ccccc2)O1
Mol. weight [g/mol]: 278.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	4.817		Crippen Method
rinpol	1715.00		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=R115381&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/45-140-6/Ethanediol-1-phenyl-DTBS.pdf>

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