

Phenol, 2,4-bis-(1,1-dimethylethyl), TMS

Inchi: InChI=1S/C17H30OSi/c1-16(2,3)13-10-14(17(4,5)6)12-15(11-13)18-19(7,8)9/h10-12H,1-
InchiKey: PNVRMDDGELICSY-UHFFFAOYSA-N
Formula: C17H30OSi
SMILES: CC(C)(C)c1cc(O[Si](C)(C)C)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 278.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	5.495		Crippen Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R58365&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/18-085-8/Phenol-2-4-bis-1-1-dimethylethyl-TMS.pdf>

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