Phenol, 3,4-dimethyl, TMS

Inchi: InChI=1S/C11H18OSi/c1-9-6-7-11(8-10(9)2)12-13(3,4)5/h6-8H,1-5H3
InchiKey: HUJKPJDYBJPESM-UHFFFAOYSA-N
Formula: C11H18OSi
SMILES: Cc1ccc(O[Si](C)(C)C)cc1C
Mol. weight [g/mol]: 194.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	3.517		Crippen Method
rinpol	1244.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1244.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R10856&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices