4-Chlorophenol, tert-butyldimethylsilyl ether

Other names:	4-chlorophenol, TBDMS
	4-Chloro-1-dimethyl(tert-butyl)silyloxybenzene
Inchi:	InChI=1S/C12H19ClOSi/c1-12(2,3)15(4,5)14-11-8-6-10(13)7-9-11/h6-9H,1-5H3
InchiKey:	GIJYKQZUGLZCKZ-UHFFFAOYSA-N
Formula:	C12H19ClOSi
SMILES:	CC(C)(C)[Si](C)(C)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	242.82
CAS:	126644-72-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	4.724		Crippen Method
rinpol	1481.10		NIST Webbook
rinpol	1481.10		NIST Webbook
rinpol	1456.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126644722&Units=SI

Legend

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