

4-Chloro-3-methylphenol, tert-butyldimethylsilyl ether

Other names:	4-chloro-3-methylphenol , TBDMS 4-Chloro-3-methylphenol, tbdms derivative
Inchi:	InChI=1S/C13H21ClOSi/c1-10-9-11(7-8-12(10)14)15-16(5,6)13(2,3)4/h7-9H,1-6H3
InchiKey:	VYYHAUWKROQSHK-UHFFFAOYSA-N
Formula:	C13H21ClOSi
SMILES:	<chem>Cc1cc(O[Si](C)(C)C(C)(C)C)ccc1Cl</chem>
Mol. weight [g/mol]:	256.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	5.032		Crippen Method
rinpola	1563.50		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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