

2,3-Dimethylphenol, trimethylsilyl ether

Other names:	2,3-Dimethylphenol, TMS Phenol, 2,3-dimethyl, TMS 2,3-Dimethylphenol, TMS ether 2,3-Dimethylphenol, tms derivative
Inchi:	InChI=1S/C11H18OSi/c1-9-7-6-8-11(10(9)2)12-13(3,4)5/h6-8H,1-5H3
InchiKey:	CXMPXUMNFRWCYIY-UHFFFAOYSA-N
Formula:	C11H18OSi
SMILES:	<chem>Cc1cccc(O[Si](C)(C)C)c1C</chem>
Mol. weight [g/mol]:	194.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	3.517		Crippen Method
rinpola	1254.60		NIST Webbook
rinpola	1252.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/78-906-0/2-3-Dimethylphenol-trimethylsilyl-ether.pdf>

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