

2,5-Dimethylbenzenethiol, S-(tert-butyl dimethylsilyl)-

Other names:	2,5-Dimethylbenzenethiol, tbdms derivative
Inchi:	InChI=1S/C14H24SSi/c1-11-8-9-12(2)13(10-11)15-16(6,7)14(3,4)5/h8-10H,1-7H3
InchiKey:	QMSWNBLVKUUYDD-UHFFFAOYSA-N
Formula:	C14H24SSi
SMILES:	<chem>Cc1ccc(C)c(S[Si](C)(C)C(C)(C)C)c1</chem>
Mol. weight [g/mol]:	252.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	5.401		Crippen Method
rinpol	1647.40		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353019&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/48-731-7/2-5-Dimethylbenzenethiol-S-tert-butyl dimethylsilyl.pdf>

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