

4-Isopropylbenzenethiol, S-(tert-butyl dimethylsilyl)-

Other names:	4-Isopropylbenzenethiol, tbdms derivative
Inchi:	InChI=1S/C15H26SSi/c1-12(2)13-8-10-14(11-9-13)16-17(6,7)15(3,4)5/h8-12H,1-7H3
InchiKey:	ZDNDUCHDMIXJKU-UHFFFAOYSA-N
Formula:	C15H26SSi
SMILES:	CC(C)c1ccc(S[Si](C)(C)C(C)(C)C)cc1
Mol. weight [g/mol]:	266.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	5.907		Crippen Method
rinsol	1734.40		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353050&Units=SI

Legend

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

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