

2-Isopropylbenzenethiol, S-(tert-butyldimethylsilyl)-

Other names:	2-Isopropylbenzenethiol, tbdms derivative
Inchi:	InChI=1S/C15H26SSi/c1-12(2)13-10-8-9-11-14(13)16-17(6,7)15(3,4)5/h8-12H,1-7H3
InchiKey:	HJQGSWKXRCBXDZ-UHFFFAOYSA-N
Formula:	C15H26SSi
SMILES:	CC(C)c1ccccc1S[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	266.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	5.907		Crippen Method
rinpol	1667.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353045&Units=SI

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/67-860-3/2-Isopropylbenzenethiol-S-tert-butyldimethylsilyl.pdf>

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