

2-Isopropylbenzenethiol, S-trimethylsilyl-

Other names:	2-Isopropylbenzenethiol, tms derivative
Inchi:	InChI=1S/C12H20SSi/c1-10(2)11-8-6-7-9-12(11)13-14(3,4)5/h6-10H,1-5H3
InchiKey:	VMRPHIVWFJYIAT-UHFFFAOYSA-N
Formula:	C12H20SSi
SMILES:	CC(C)c1ccccc1S[Si](C)(C)C
Mol. weight [g/mol]:	224.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	4.737		Crippen Method
rinpol	1433.80		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/85-027-8/2-Isopropylbenzenethiol-S-trimethylsilyl.pdf>

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