

2-Methylbenzenethiol, S-trimethylsilyl-

Other names:	2-Methylbenzenethiol, tms derivative
Inchi:	InChI=1S/C10H16SSi/c1-9-7-5-6-8-10(9)11-12(2,3)4/h5-8H,1-4H3
InchiKey:	UEULRLVZLDCRFT-UHFFFAOYSA-N
Formula:	C10H16SSi
SMILES:	Cc1ccccc1S[Si](C)(C)C
Mol. weight [g/mol]:	196.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	3.922		Crippen Method
rinpol	1326.90		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353010&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/86-012-3/2-Methylbenzenethiol-S-trimethylsilyl.pdf>

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