

2,5-Dimethylbenzenethiol, S-trimethylsilyl-

Other names:	2,5-Dimethylbenzenethiol, tms derivative
Inchi:	InChI=1S/C11H18SSi/c1-9-6-7-10(2)11(8-9)12-13(3,4)5/h6-8H,1-5H3
InchiKey:	HATDGCWADKWNFX-UHFFFAOYSA-N
Formula:	C11H18SSi
SMILES:	<chem>Cc1ccc(C)c(S[Si](C)(C)C)c1</chem>
Mol. weight [g/mol]:	210.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	4.230		Crippen Method
rinpol	1401.60		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=U353020&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/50-539-8/2-5-Dimethylbenzenethiol-S-trimethylsilyl.pdf>

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