

3-Methoxythiophenol, S-trimethylsilyl-

Other names:	3-Methoxythiophenol, tms derivative
Inchi:	InChI=1S/C10H16OSSi/c1-11-9-6-5-7-10(8-9)12-13(2,3)4/h5-8H,1-4H3
InchiKey:	NTXJOZBRSRPSJD-UHFFFAOYSA-N
Formula:	C10H16OSSi
SMILES:	COc1cccc(S[Si](C)(C)C)c1
Mol. weight [g/mol]:	212.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	3.622		Crippen Method
rinpol	1470.40		NIST Webbook
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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=U352997&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/94-518-3/3-Methoxythiophenol-S-trimethylsilyl.pdf>

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