

2-Methoxy-5-nitrophenol, trimethylsilyl ether

Other names:	2-Methoxy-5-nitrophenol, tms derivative
Inchi:	InChI=1S/C10H15NO4Si/c1-14-9-6-5-8(11(12)13)7-10(9)15-16(2,3)4/h5-7H,1-4H3
InchiKey:	XPRNUJURPHIMGP-UHFFFAOYSA-N
Formula:	C10H15NO4Si
SMILES:	COc1ccc([N+](=O)[O-])cc1O[Si](C)(C)C
Mol. weight [g/mol]:	241.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	2.817		Crippen Method
rinpol	1697.90		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352892&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/59-847-7/2-Methoxy-5-nitrophenol-trimethylsilyl-ether.pdf>

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