

m-Anisic acid, 4-(trimethylsiloxy)-, methyl ester

Other names:	Methyl 3-methoxy-4-[(trimethylsilyl)oxy]benzoate Methyl vanillate, trimethylsilyl ether Benzoic acid, 3-methoxy-4-[(trimethylsilyl)oxy]-, methyl ester Methyl vanillate, tms derivative
Inchi:	InChI=1S/C12H18O4Si/c1-14-11-8-9(12(13)15-2)6-7-10(11)16-17(3,4)5/h6-8H,1-5H3
InchiKey:	NWDAPAUUGXPOJ-UHFFFAOYSA-N
Formula:	C12H18O4Si
SMILES:	<chem>COC(=O)c1ccc(O[Si](C)(C)C)c(OC)c1</chem>
Mol. weight [g/mol]:	254.35
CAS:	27798-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	2.696		Crippen Method
rinsol	1652.60		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27798534&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinsol:	Non-polar retention indices

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