Benzoic acid, 3-methoxy-4-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	m-Anisic acid, 4-(trimethylsiloxy)-, trimethylsilyl ester
	4,7-Bis(trimethylsilyl)vanillic acid
	Vanillic acid, trimethylsiloxytrimethylsilyl ester
	4-TMS-Oxy-3-methoxybenzoic acid, TMS ester
	Vanillic acid, bis-TMS
	Vanillic acid, di-TMS
	Vanillic acid, TMS
	Vanillic acid, 2tms derivative
Inchi:	InChI=1S/C14H24O4Si2/c1-16-13-10-11(14(15)18-20(5,6)7)8-9-12(13)17-19(2,3)4/h8-10
InchiKey:	UQZKEPFYTGMPKU-UHFFFAOYSA-N
Formula:	C14H24O4Si2
SMILES:	COc1cc(C(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	312.51
CAS:	2078-15-1

Physical Properties

Property code	Value	Unit	Source
log10ws	0.27		Crippen Method
logp	3.901		Crippen Method
rinpol	1754.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1754.00		NIST Webbook

rinpol	1755.00	NIST Webbook
rinpol	1754.00	NIST Webbook
rinpol	1753.00	NIST Webbook
rinpol	1754.00	NIST Webbook
rinpol	1754.00	NIST Webbook
rinpol	1774.00	NIST Webbook
rinpol	1776.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1774.00	NIST Webbook
rinpol	1776.00	NIST Webbook
rinpol	1774.00	NIST Webbook
rinpol	1754.00	NIST Webbook
rinpol	1781.00	NIST Webbook
rinpol	1779.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078151&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices