Benzoic acid, 3-methoxy-, trimethylsilyl ester

Other names:	Benzoic acid, 3-methoxy, TMS
Inchi:	InChI=1S/C11H16O3Si/c1-13-10-7-5-6-9(8-10)11(12)14-15(2,3)4/h5-8H,1-4H3
InchiKey:	PPUSJGXNIQTKKU-UHFFFAOYSA-N
Formula:	C11H16O3Si
SMILES:	COc1cccc(C(=O)O[Si](C)(C)C)c1
Mol. weight [g/mol]:	224.33
CAS:	959111-51-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Crippen Method
logp	2.687		Crippen Method
rinpol	1485.00		NIST Webbook
rinpol	1455.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959111514&Units=SI

Legend

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

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