tert-Butyldimethylsilyl 3-methylbenzoate

Other names:	Benzoic acid, 3-methyl-, tert-butyldimethylsilyl ester
Inchi:	InChI=1S/C14H22O2Si/c1-11-8-7-9-12(10-11)13(15)16-17(5,6)14(2,3)4/h7-10H,1-6H3
InchiKey:	KQMQUHOKNQDKJF-UHFFFAOYSA-N
Formula:	C14H22O2Si
SMILES:	Cc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	250.41
CAS:	959296-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	4.157		Crippen Method
rinpol	1587.00		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=C959296298&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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