Silanol, (1,1-dimethylethyl)dimethyl-, benzoate

Other names:	Benzoic acid, tert-butyldimethylsilyl ester
	Benzoic acid, DMTBS
	Benzoic acid, TBDMS
	tert-Butyldimethylsilyl benzoate
	Benzoic acid, tbdms derivative
Inchi:	InChI=1S/C13H20O2Si/c1-13(2,3)16(4,5)15-12(14)11-9-7-6-8-10-11/h6-10H,1-5H3
InchiKey:	GPSVOHKZRIFVOF-UHFFFAOYSA-N
Formula:	C13H20O2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1
Mol. weight [g/mol]:	236.38
CAS:	75732-41-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.86		Crippen Method
logp	3.849		Crippen Method
rinpol	1508.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1484.61		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1488.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75732411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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