(3,3,5-Trimethylcyclohexyl) 2-(tert-butyldimethylsilyloxy)benzoate

Other names:	Benzoic acid, 2-(tert-butyldimethylsilyl)oxy-, 3,3,5-trimethylcyclohexyl ester
Inchi:	InChI=1S/C22H36O3Si/c1-16-13-17(15-22(5,6)14-16)24-20(23)18-11-9-10-12-19(18)25-
InchiKey:	OMMMDJPXMYYIHB-UHFFFAOYSA-N
Formula:	C22H36O3Si
SMILES:	CC1CC(OC(=O)c2ccccc2O[Si](C)(C)C(C)(C)C)CC(C)(C)C1
Mol. weight [g/mol]:	376.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	6.442		Crippen Method
rinpol	2242.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373291&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

Latest version available from:
https://www.chemeo.com/cid/37-957-9/3-3-5-Trimethylcyclohexyl-2-tert-butyldimethylsilyloxy-benzoate.pdf
Generated by Cheméo on 2024-10-12 02:28:15.222439885 +0000 UTC m=+3280957.859409143.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.