(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: 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=U373291&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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