

(3,3,5-Trimethylcyclohexyl) 2-trimethylsilyloxybenzoate

Other names:	Benzoic acid, 2-trimethylsilyloxy-, 3,3,5-trimethylcyclohexyl ester
Inchi:	InChI=1S/C19H30O3Si/c1-14-11-15(13-19(2,3)12-14)21-18(20)16-9-7-8-10-17(16)22-23
InchiKey:	XGJLZWZTLVNTRV-UHFFFAOYSA-N
Formula:	C19H30O3Si
SMILES:	CC1CC(OC(=O)c2ccccc2O[Si](C)(C)C)CC(C)(C)C1
Mol. weight [g/mol]:	334.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	5.272		Crippen Method
rinpol	1998.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373063&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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