Benzoic acid, 4-trifluoroacetyloxy-, trimethylsilyl ester

Inchi: InChI=1S/C12H13F3O4Si/c1-20(2,3)19-10(16)8-4-6-9(7-5-8)18-11(17)12(13,14)15/h4-7H
InchiKey: HDAXALAOLGSNFT-UHFFFAOYSA-N
Formula: C12H13F3O4Si
SMILES: C[Si](C)(C)OC(=O)c1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 306.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	3.146		Crippen Method
rinpol	1367.00		NIST Webbook
rinpol	1367.00		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=U375048&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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