3-Trifluoroacetyloxybenzoic acid, 3-(trimethylsilyloxycarbonyl)phenyl ester

Inchi: InChI=1S/C19H17F3O6Si/c1-29(2,3)28-17(24)13-7-5-8-14(11-13)26-16(23)12-6-4-9-15(1

InchiKey: OHZJAIZULNFHTO-UHFFFAOYSA-N

Formula: C19H17F3O6Si

SMILES: C[Si](C)(C)OC(=O)c1cccc(OC(=O)c2cccc(OC(=O)C(F)(F)F)c2)c1

Mol. weight [g/mol]: 426.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	4.365		Crippen Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		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=U375019&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices