Benzoic acid, 2-heptafluuorobutyryloxy-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F7O4Si/c1-26(2,3)25-10(22)8-6-4-5-7-9(8)24-11(23)12(15,16)13(17,18

InchiKey: FYJONWYIRGBNEX-UHFFFAOYSA-N

Formula: C14H13F7O4Si

SMILES: C[Si](C)(C)OC(=O)c1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 406.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.417		Crippen Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375211&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