Benzoic acid, 3-heptafluorobutyryloxy-, trimethylsilyl ester

Inchi: InChI=1S/C14H13F7O4Si/c1-26(2,3)25-10(22)8-5-4-6-9(7-8)24-11(23)12(15,16)13(17,18
InchiKey: KBWXVIOHTOGUNJ-UHFFFAOYSA-N
Formula: C14H13F7O4Si
SMILES: C[Si](C)(C)OC(=O)c1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 406.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	4.417		Crippen Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		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=U375031&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices