Benzoic acid DMPFPS

Inchi: InChI=1S/C15H11F5O2Si/c1-23(2,22-15(21)8-6-4-3-5-7-8)14-12(19)10(17)9(16)11(18)13

InchiKey: XFSCDBAEBTZUMW-UHFFFAOYSA-N

Formula: C15H11F5O2Si

SMILES: C[Si](C)(OC(=O)c1ccccc1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 346.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.43		Crippen Method
logp	3.651		Crippen Method
rinpol	1690.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R102499&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices