Benzoic acid, 4-pentafluoropropionylthio-, trimethylsilyl ester

Inchi: InChI=1S/C13H13F5O3SSi/c1-23(2,3)21-10(19)8-4-6-9(7-5-8)22-11(20)12(14,15)13(16,1

InchiKey: CEOTUOSURZYRMP-UHFFFAOYSA-N

Formula: C13H13F5O3SSi

SMILES: C[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 372.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Crippen Method
logp	4.495		Crippen Method
rinpol	1563.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375189&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

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