Benzoic acid, 2-heptafluorobutyrylthio-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C17H19F7O3SSi/c1-14(2,3)29(4,5)27-12(25)10-8-6-7-9-11(10)28-13(26)15(18
InchiKey: VAXQKLHLZLAZSG-UHFFFAOYSA-N
Formula: C17H19F7O3SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 464.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	6.300		Crippen Method
rinpol	1746.00		NIST Webbook
rinpol	1746.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375196&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