

# Benzoic acid, 2-pentafluoropropionylthio-, tert.-butyldimethylsilyl ester

**Inchi:** InChI=1S/C16H19F5O3SSi/c1-14(2,3)26(4,5)24-12(22)10-8-6-7-9-11(10)25-13(23)15(17)  
**InchiKey:** RDUIIDQTASIGGK-UHFFFAOYSA-N  
**Formula:** C16H19F5O3SSi  
**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)C(F)(F)F  
**Mol. weight [g/mol]:** 414.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	5.665		Crippen Method
rinpol	1720.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375197&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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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