

# Benzoic acid, 3-trifluoroacetylthio-, tert.-butyldimethylsilyl ester

**Inchi:** InChI=1S/C15H19F3O3SSi/c1-14(2,3)23(4,5)21-12(19)10-7-6-8-11(9-10)22-13(20)15(16)  
**InchiKey:** FLCOVQSEAZPHKF-UHFFFAOYSA-N  
**Formula:** C15H19F3O3SSi  
**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)F)c1  
**Mol. weight [g/mol]:** 364.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	5.030		Crippen Method
rinpol	1746.00		NIST Webbook

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375168&Units=SI>

## Legend

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

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