

# Benzoic acid, 4-trifluoroacetylthio-, tert.-butyldimethylsilyl ester

**Inchi:** InChI=1S/C15H19F3O3SSi/c1-14(2,3)23(4,5)21-12(19)10-6-8-11(9-7-10)22-13(20)15(16)  
**InchiKey:** QCPFBHPSCWKMLZ-UHFFFAOYSA-N  
**Formula:** C15H19F3O3SSi  
**SMILES:** CC(C)(C)[Si](C)(C)OC(=O)c1ccc(SC(=O)C(F)(F)F)cc1  
**Mol. weight [g/mol]:** 364.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	5.030		Crippen Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375183&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/114-815-0/Benzoic-acid-4-trifluoroacetylthio-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-28 17:32:40.55105965 +0000 UTC m=+16614809.471636961.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.