

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

Inchi: InChI=1S/C15H19F3O3SSi/c1-14(2,3)23(4,5)21-12(19)10-8-6-7-9-11(10)22-13(20)15(16)
InchiKey: YCXIWNNFRNKRKA-UHFFFAOYSA-N
Formula: C15H19F3O3SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)F
Mol. weight [g/mol]: 364.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	5.030		Crippen Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375198&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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

Latest version available from:

<https://www.cheméo.com/cid/113-572-1/Benzoic-acid-2-trifluoroacetylthio-tert-butyldimethylsilyl-ester.pdf>

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