Benzoic acid, 3-trifluoroacetylthio-, trimethylsilyl ester

Inchi: InChI=1S/C12H13F3O3SSi/c1-20(2,3)18-10(16)8-5-4-6-9(7-8)19-11(17)12(13,14)15/h4-7

InchiKey: XHLBNQMTZDRIFX-UHFFFAOYSA-N

Formula: C12H13F3O3SSi

SMILES: C[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)F)c1

Mol. weight [g/mol]: 322.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	3.859		Crippen Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375174&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices