

Benzoic acid, 2-trifluoroacetylthio-, trimethylsilyl ester

Inchi: InChI=1S/C12H13F3O3SSi/c1-20(2,3)18-10(16)8-6-4-5-7-9(8)19-11(17)12(13,14)15/h4-7
InchiKey: FLJPYIKVOUXNLO-UHFFFAOYSA-N
Formula: C12H13F3O3SSi
SMILES: C[Si](C)(C)OC(=O)c1ccccc1SC(=O)C(F)(F)F
Mol. weight [g/mol]: 322.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	3.859		Crippen Method
rinpol	1504.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375204&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/14-723-3/Benzoic-acid-2-trifluoroacetylthio-trimethylsilyl-ester.pdf>

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