

2-(Trifluoromethyl)thiophenol, S-(tert-butyldimethylsilyl)-

Inchi: InChI=1S/C13H19F3SSi/c1-12(2,3)18(4,5)17-11-9-7-6-8-10(11)13(14,15)16/h6-9H,1-5H3
InchiKey: ZEMWGAQLGJIFRN-UHFFFAOYSA-N
Formula: C13H19F3SSi
SMILES: CC(C)(C)[Si](C)(C)Sc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 292.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	5.803		Crippen Method
rinpol	1517.90		NIST Webbook
rinpol	1517.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U353096&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/47-821-8/2-Trifluoromethyl-thiophenol-S-tert-butyldimethylsilyl.pdf>

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