

Benzoic acid, 3-pentafluoropropionylthio-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C16H19F5O3SSi/c1-14(2,3)26(4,5)24-12(22)10-7-6-8-11(9-10)25-13(23)15(17)
InchiKey: KKUJCVLFTOXYQO-UHFFFAOYSA-N
Formula: C16H19F5O3SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(SC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 414.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	5.665		Crippen Method
rinpol	1742.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375167&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

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<https://www.chemeo.com/cid/35-932-8/Benzoic-acid-3-pentafluoropropionylthio-tert-butyldimethylsilyl-ester.pdf>

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