

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

Inchi: InChI=1S/C16H19F5O4Si/c1-14(2,3)26(4,5)25-12(22)10-7-6-8-11(9-10)24-13(23)15(17,18)21
InchiKey: IJTVPTVEYXGBEC-UHFFFAOYSA-N
Formula: C16H19F5O4Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 398.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	4.952		Crippen Method
rinsol	1566.00		NIST Webbook
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Sources

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375029&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
rinsol: Non-polar retention indices

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<https://www.cheméo.com/cid/119-109-9/Benzoic-acid-3-pentafluoropropionyloxy-tert-butyldimethylsilyl-ester.pdf>

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