

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

Inchi: InChI=1S/C13H20O3Si/c1-13(2,3)17(4,5)16-12(15)10-7-6-8-11(14)9-10/h6-9,14H,1-5H3
InchiKey: ZNWANTDZMJTLBH-UHFFFAOYSA-N
Formula: C13H20O3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cccc(O)c1
Mol. weight [g/mol]: 252.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	3.554		Crippen Method
rinpol	1806.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374548&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/17-624-0/Benzoic-acid-3-hydroxy-tert-butyldimethylsilyl-ester.pdf>

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