

Benzoic acid, 2-(tert.-butyldimethylsilyloxy)-, methyl ester

Inchi: InChI=1S/C14H22O3Si/c1-14(2,3)18(5,6)17-12-10-8-7-9-11(12)13(15)16-4/h7-10H,1-6H3
InchiKey: PAJWOPJNPUYXFC-UHFFFAOYSA-N
Formula: C14H22O3Si
SMILES: COC(=O)c1ccccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 266.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.98		Crippen Method
logp	3.857		Crippen Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374491&Units=SI>

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/40-488-6/Benzoic-acid-2-tert-butyldimethylsilyloxy-methyl-ester.pdf>

Generated by Cheméo on 2024-04-20 14:04:29.402701465 +0000 UTC m=+15911118.323278776.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.