

Benzoic acid, 2-acetyloxy-, tert.-butyldimethylsilyl ester

Inchi: InChI=1S/C15H22O4Si/c1-11(16)18-13-10-8-7-9-12(13)14(17)19-20(5,6)15(2,3)4/h7-10H
InchiKey: PTUZUDDOZGCNTE-UHFFFAOYSA-N
Formula: C15H22O4Si
SMILES: CC(=O)Oc1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 294.42
CAS: 129512-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	3.774		Crippen Method
rinpole	1752.00		NIST Webbook
rinpole	1790.80		NIST Webbook
rinpole	1752.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C129512443&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
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-039-2/Benzoic-acid-2-acetyloxy-tert-butyldimethylsilyl-ester.pdf>

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