

Benzoic acid, 4-acetyloxy-, trimethylsilyl ester

Inchi: InChI=1S/C12H16O4Si/c1-9(13)15-11-7-5-10(6-8-11)12(14)16-17(2,3)4/h5-8H,1-4H3
InchiKey: WBHIDAUSERADOK-UHFFFAOYSA-N
Formula: C12H16O4Si
SMILES: CC(=O)Oc1ccc(C(=O)O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 252.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	2.604		Crippen Method
rinpol	1688.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375073&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

Latest version available from:

<https://www.chemeo.com/cid/11-011-6/Benzoic-acid-4-acetyloxy-trimethylsilyl-ester.pdf>

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