

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

Inchi: InChI=1S/C14H22O3Si/c1-14(2,3)18(5,6)17-13(15)11-8-7-9-12(10-11)16-4/h7-10H,1-6H3
InchiKey: JQBGDLLYGSUWMZ-UHFFFAOYSA-N
Formula: C14H22O3Si
SMILES: COc1cccc(C(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 266.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.98 | | Crippen Method |
| logp | 3.857 | | Crippen Method |
| rinpol | 1724.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374506&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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