

3,4-Dimethylbenzoic acid, tert-butyldimethylsilyl ester

Other names: 3,4-Dimethylbenzoic acid, tBDMS
Inchi: InChI=1S/C15H24O2Si/c1-11-8-9-13(10-12(11)2)14(16)17-18(6,7)15(3,4)5/h8-10H,1-7H3
InchiKey: MUUQEDUNJLHIPK-UHFFFAOYSA-N
Formula: C15H24O2Si
SMILES: Cc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1C
Mol. weight [g/mol]: 264.44

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.81 | | Crippen Method |
| logp | 4.465 | | Crippen Method |
| rinpol | 1730.00 | | NIST Webbook |
| rinpol | 1730.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373235&Units=SI>

Legend

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

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