

# 3-Hydroxy-4-methoxybenzoic acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl ester

Other names: Isovanillic acid, 2-bromo derivative

Inchi: InChI=1S/C20H36O4Si2/c1-19(2,3)25(8,9)23-17-14-15(12-13-16(17)22-7)18(21)24-26(10,11)

InchiKey: HDAZAUCOLZBZFH-UHFFFAOYSA-N

Formula: C20H36O4Si2

SMILES: COc1ccc(C(=O)O[Si](C)(C)C(C)(C)C)cc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 396.67

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.24   |      | Crippen Method |
| logp          | 6.241   |      | Crippen Method |
| rinpol        | 2226.90 |      | NIST Webbook   |
| rinpol        | 2226.90 |      | NIST Webbook   |

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352852&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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