

# Benzeneacetic acid, 4-[(tert-butyldimethylsilyl)oxy]-3-methoxy-, tert-butyldimethylsilyl ester

Other names: Homovanillic acid, 4-tert-butyldimethylsilyloxy-, tert-butyldimethylsilyl ester  
Homovanillic acid, diTBDMS

Phenylacetic acid, 4-hydroxy-3-methoxy, bis-TBDMS

4-Hydroxy-3-methoxyphenylacetic acid, DMTBS

Homovanillic acid, TBDMS

Phenylacetic acid, 4-hydroxy-3-methoxy, TBDMS

Homovanillic acid, 2tdms derivative

Inchi: InChI=1S/C21H38O4Si2/c1-20(2,3)26(8,9)24-17-13-12-16(14-18(17)23-7)15-19(22)25-2

InchiKey: FDHILQPZGKJPBA-UHFFFAOYSA-N

Formula: C21H38O4Si2

SMILES: COc1cc(CC(=O)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 410.69

CAS: 78324-15-9

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.08   |      | Crippen Method |
| logp          | 6.170   |      | Crippen Method |
| rinpol        | 2246.00 |      | NIST Webbook   |
| rinpol        | 2249.50 |      | NIST Webbook   |
| rinpol        | 2256.00 |      | NIST Webbook   |
| rinpol        | 2246.47 |      | NIST Webbook   |
| rinpol        | 2249.00 |      | NIST Webbook   |
| rinpol        | 2249.50 |      | NIST Webbook   |
| rinpol        | 2246.00 |      | NIST Webbook   |

## Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78324159&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

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